

Supporting Information

C-H Bond Activation of Terminal Allenes: Formation of Hydrido-Alkenylcarbyne-Osmium and Disubstituted Vinylidene-Ruthenium Derivatives

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Contents:

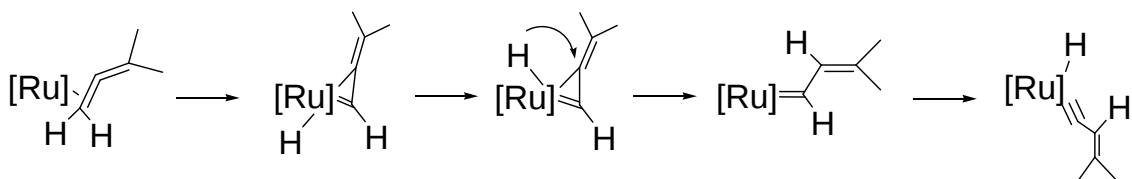
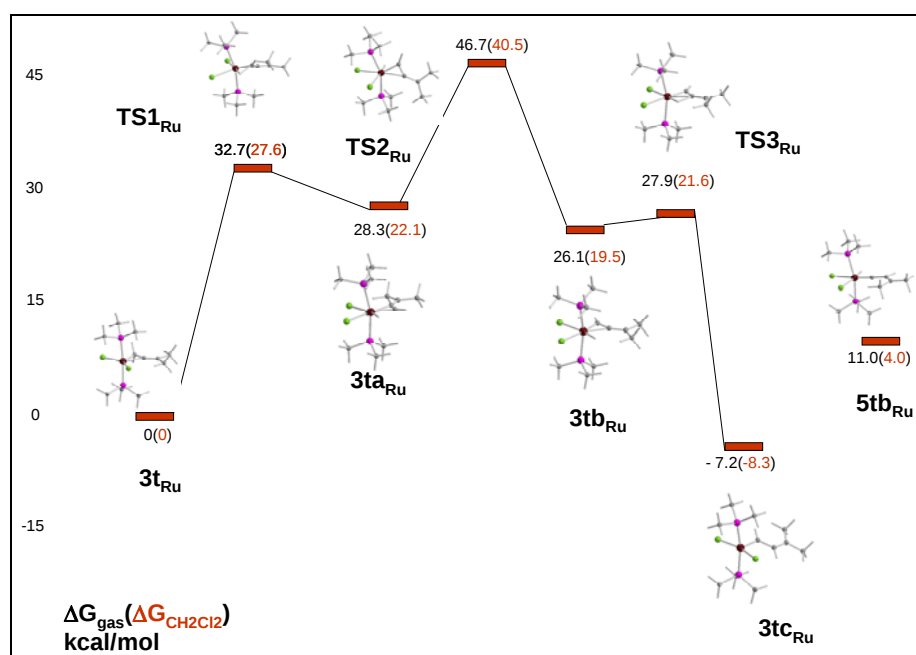
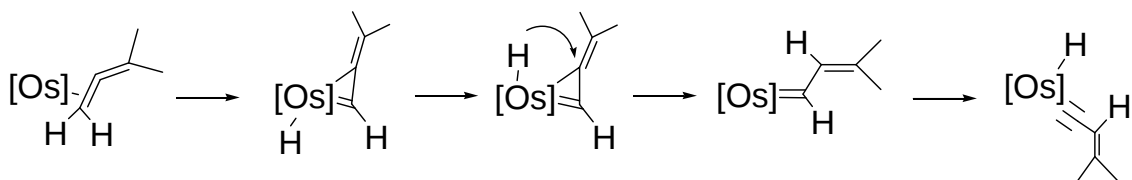
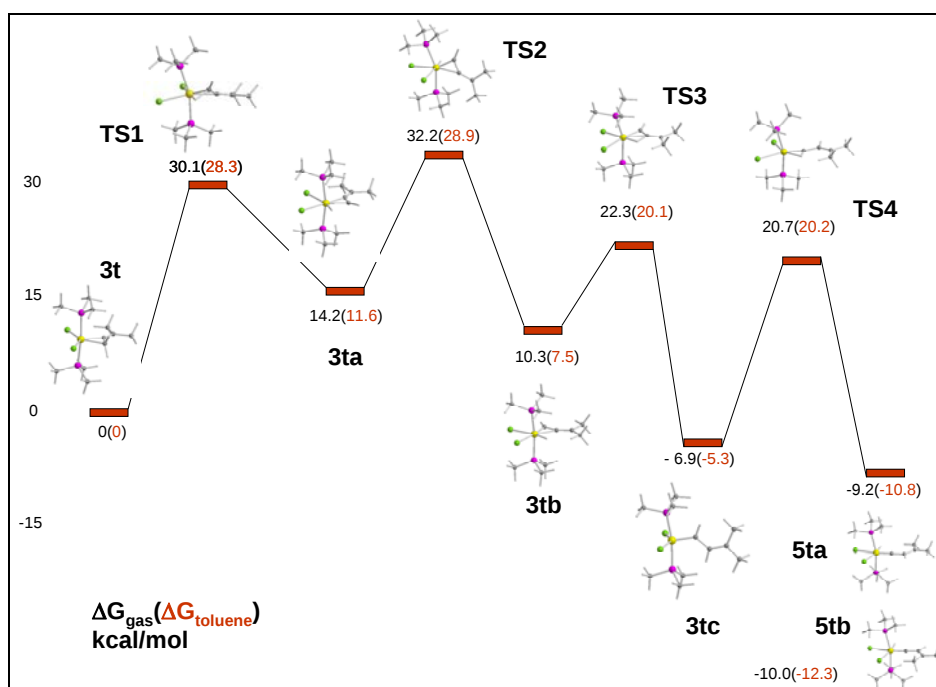
Computational details, energy pathways, cartesian coordinates of the optimized structures and calculated thermochemistry data for the species

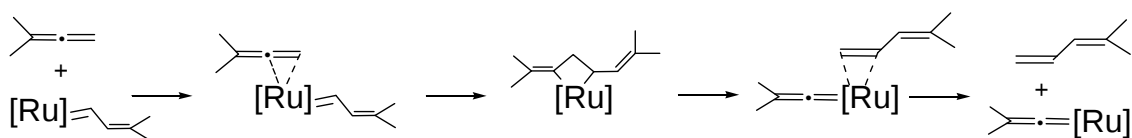
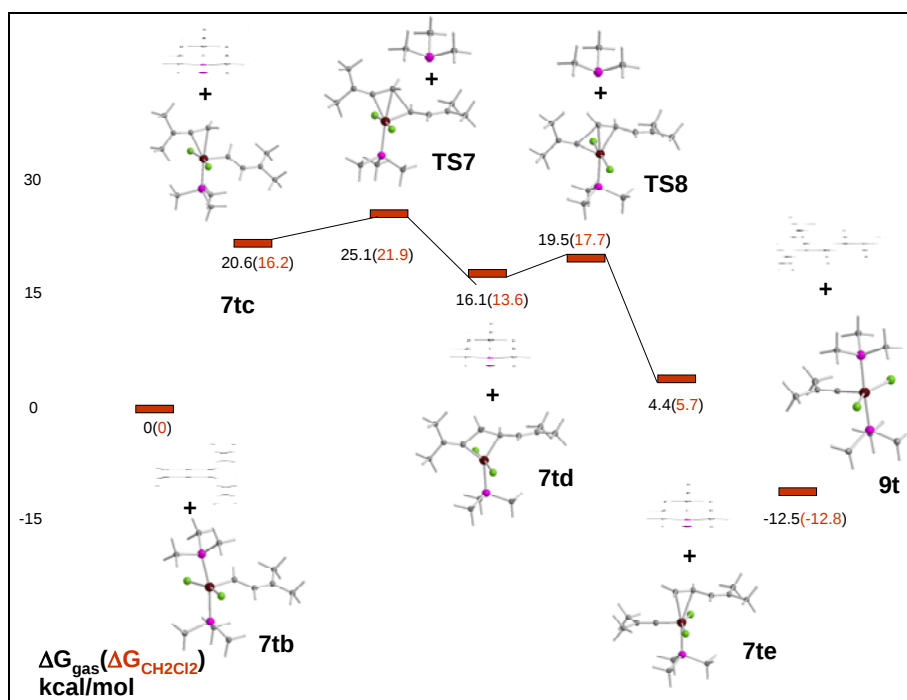
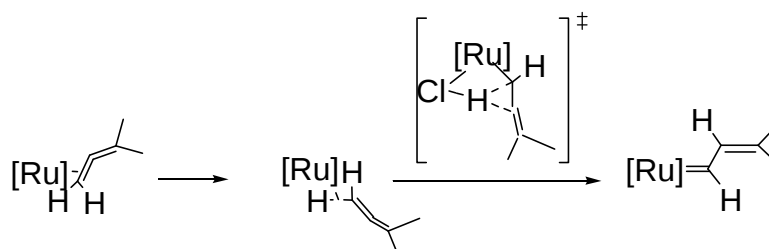
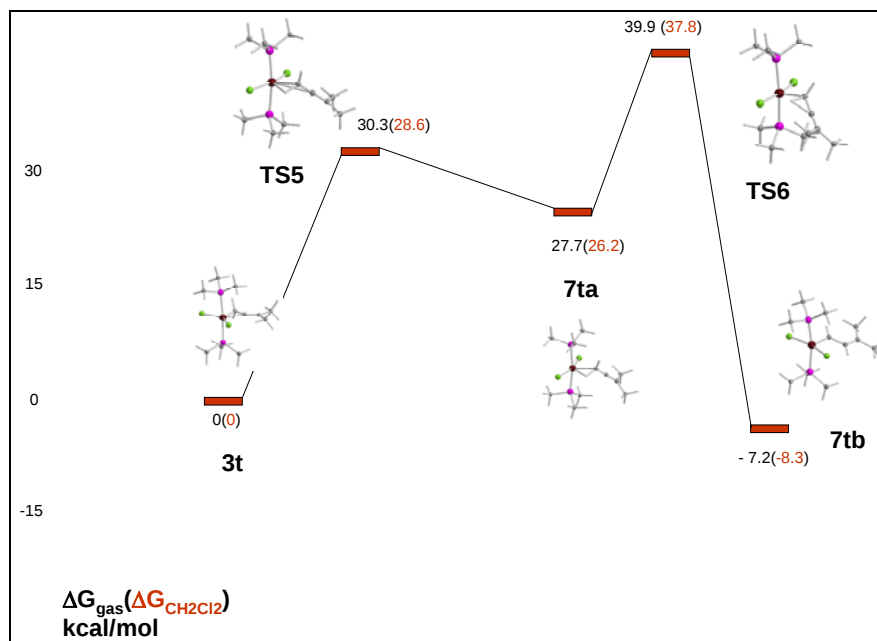
Computational details and orthogonal coordinates of the model complexes. The theoretical calculations were carried out on the model complexes by optimizing the structures at the b3pw91-DFT levels with the Gaussian 03 program.¹ The basis sets used were LANL2DZ basis and pseudopotentials for Os, and 6-31G(d,p) for the rest of atoms. The transition states have been found by carry out potential energy surfaces of the processes following the reaction coordinates, optimized the maxima, and confirmed by frequency calculations. The connections between the starting and final reactants have been checked by slightly perturbing the TS geometry towards the minima geometries and reoptimizing.

The numerical values shown in the schemes corresponds to calculated free energy (298.15 K and 1 atm)² and $\Delta G_{\text{solvent}}$ ($\Delta G_{\text{solvent}} = \Delta G_{\text{gas}} + \Delta \Delta G_{\text{solv}}$). The solvation free energies (G_{solv}) were obtained from the single-point calculations combined with the PCM models.

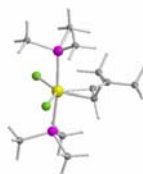
(1) Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji,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

(2) Thermochemistry in gaussian, Ochterski, J. W., Gaussian, Inc., 2000.





3t



Os	0.00004200	-0.33464500	0.00815900
P	2.36914900	-0.40887400	0.09721000
P	-2.36900300	-0.40946000	0.09725400
C	3.27000800	-0.67459900	-1.48090000
H	4.33555900	-0.84746800	-1.30212700
H	2.83682200	-1.53856100	-1.99102300
H	3.16012300	0.20240000	-2.12405600
C	3.19055800	1.05939300	0.82532400
H	2.78077300	1.22352400	1.82452400
H	4.27521400	0.92757200	0.88479100
H	2.95842800	1.93482100	0.21387200
C	2.95411400	-1.79782600	1.14659300
H	2.58950100	-2.73765100	0.72380000
H	4.04661400	-1.82390900	1.20719300
H	2.53502900	-1.67974100	2.14917600
C	-3.26971200	-0.67530700	-1.48091400
H	-4.33530600	-0.84806200	-1.30229500
H	-3.15963600	0.20160500	-2.12415900
H	-2.83653500	-1.53937500	-1.99087400
C	-3.19074200	1.05856000	0.82547600
H	-4.27530000	0.92626800	0.88562200
H	-2.78041100	1.22312800	1.82438100
H	-2.95938500	1.93394800	0.21367200
C	-2.95351900	-1.79868600	1.14652000
H	-2.53446700	-1.68057000	2.14911300
H	-4.04600900	-1.82516900	1.20711900
H	-2.58856300	-2.73832700	0.72361100
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Cl	0.00030800	-2.34899200	-1.27285900
C	-0.00020400	1.56172600	-0.76230900
C	-0.00057800	2.87123100	-0.49944500
C	-0.00071900	3.85107700	-1.65167100
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H	-0.00059300	3.34475700	-2.61996300
H	-0.88015400	4.50846200	-1.60968600
C	-0.00075500	3.49380000	0.86760800
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C	0.00001300	0.65681200	-1.86407300
H	-0.90518600	0.50459000	-2.45171100
H	0.90527400	0.50486300	-2.45167900

Zero-point correction= 0.349017 (Hartree/Particle)
 Thermal correction to Energy= 0.375809
 Thermal correction to Enthalpy= 0.376753
 Thermal correction to Gibbs Free Energy= 0.292765
 Sum of electronic and zero-point Energies= -2128.505545
 Sum of electronic and thermal Energies= -2128.478754
 Sum of electronic and thermal Enthalpies= -2128.477810
 Sum of electronic and thermal Free Energies= -2128.561798

DeltaG (solv) (kcal/mol) = 11.17

3ta

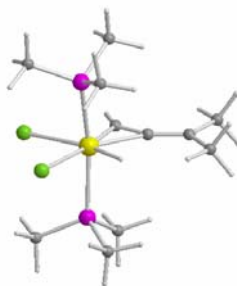


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C	3.24245000	-0.83528400	-1.70900800
H	4.32758000	-0.90062500	-1.58273400
H	2.85362400	-1.80633500	-2.02571700
H	3.01141000	-0.10130300	-2.48533200
C	3.18764300	1.21688100	0.34954600
H	2.77572400	1.49581500	1.32283600
H	4.27504600	1.11975900	0.42118900
H	2.93522200	2.00027200	-0.36898900
C	3.05145800	-1.56369900	1.07287100
H	2.70495200	-2.56307300	0.80414000
H	4.14509800	-1.52831100	1.09746900
H	2.63471700	-1.31204600	2.05024200
C	-3.05507400	-1.60093600	-1.43081200
H	-4.12337600	-1.78458900	-1.27995000
H	-2.89940900	-1.12228100	-2.40105600
H	-2.50834700	-2.54705700	-1.41779300
C	-3.36113400	0.99498000	-0.18329300
H	-4.42665800	0.77339900	-0.07068400
H	-3.04207200	1.66310200	0.62000800
H	-3.19692500	1.50265000	-1.13698800
C	-2.91371200	-1.33949800	1.43960500
H	-2.60139400	-0.72486400	2.28573600
H	-4.00037700	-1.46951900	1.43548600
H	-2.41344000	-2.30651100	1.52307500
Cl	0.14609000	-0.03967100	2.22910500
Cl	0.02213600	-2.70697500	0.11620800
C	-0.08957200	1.84259700	-0.44319400
C	-0.17897900	3.09817600	0.04816800
C	-0.25687300	4.27865400	-0.88368200
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H	-0.21190200	3.98539100	-1.93528800
H	-1.18671000	4.84158400	-0.72350000
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C	-0.02251900	1.13913000	-1.60039600
H	0.02277200	-0.95872600	-1.72049100
H	0.02178200	1.26693800	-2.67671900

Zero-point correction= 0.346292 (Hartree/Particle)
 Thermal correction to Energy= 0.373062
 Thermal correction to Enthalpy= 0.374006
 Thermal correction to Gibbs Free Energy= 0.290094
 Sum of electronic and zero-point Energies= -2128.483030
 Sum of electronic and thermal Energies= -2128.456260
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DeltaG (solv) (kcal/mol) = 8.59

3tb

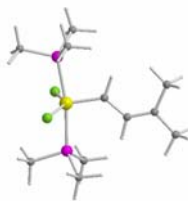


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P	2.37400000	-0.35498300	0.17654700
P	-2.37373800	-0.35591800	0.17653200
C	3.36892700	0.86047500	-0.77557500
H	3.03447100	1.87321400	-0.53739500
H	4.43378900	0.76577600	-0.54302200
H	3.21734400	0.68492100	-1.84367100
C	2.94371100	-0.12883300	1.90169300
H	2.39420200	-0.83212700	2.53166100
H	4.01954300	-0.30861400	1.99216100
H	2.71347100	0.88792100	2.22921600
C	3.04732800	-1.97643200	-0.32043700
H	4.13254600	-2.00787900	-0.18284600
H	2.56387500	-2.74437800	0.28707500
H	2.78198800	-2.16152700	-1.36321200
C	-3.04627700	-1.97845900	-0.31795000
H	-2.56321400	-2.74515900	0.29143400
H	-4.13160800	-2.00983100	-0.18123000
H	-2.77999700	-2.16543400	-1.36015400
C	-3.36915700	0.85748800	-0.77768000
H	-3.21752400	0.68006700	-1.84546000
H	-4.43397800	0.76279800	-0.54492100
H	-3.03509800	1.87077400	-0.54129700
C	-2.94371800	-0.12735200	1.90128100
H	-2.71346600	0.88984000	2.22742900
H	-4.01956800	-0.30695500	1.99188200
H	-2.39434500	-0.82980900	2.53230800
Cl	0.00003100	-1.82771100	-1.94832000
Cl	0.00046900	-2.10206300	1.47636000
C	0.00005900	1.10960900	-1.50861100
H	-0.00003200	1.08875700	-2.59209200
C	-0.00016600	1.91241400	-0.41306600
C	-0.00080200	3.17410900	0.06111900
C	-0.00154200	3.50427400	1.52258200
H	-0.87971600	4.10860400	1.78915600
H	-0.00089500	2.60287400	2.13886200
H	0.87531600	4.11026800	1.78969900
C	-0.00081800	4.34268200	-0.88865700
H	0.87758900	4.98175300	-0.72512200
H	-0.00024100	4.02237600	-1.93299900
H	-0.87984600	4.98110000	-0.72589500

Zero-point correction= 0.346037 (Hartree/Particle)
 Thermal correction to Energy= 0.372803
 Thermal correction to Enthalpy= 0.373748
 Thermal correction to Gibbs Free Energy= 0.289692
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DeltaG (solv) (kcal/mol) = 8.39

3tc

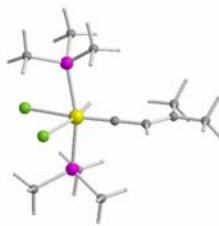


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H	-3.18649200	-2.85527100	1.39954600
H	-1.93288800	-2.00687800	2.35392000
H	-3.17374700	-1.07561100	1.50472300
C	-2.54490700	-1.97137400	-1.45134100
H	-1.92994600	-2.01209900	-2.35366600
H	-3.18521900	-2.85746300	-1.39880400
H	-3.17135100	-1.07806500	-1.50835700
C	-0.65974000	-3.55376200	0.00222800
H	-0.03182000	-3.65417100	0.89155800
H	-1.41971700	-4.34164600	0.00211300
H	-0.03018500	-3.65547200	-0.88579700
C	2.60743700	2.09141900	1.44297400
H	3.58749000	2.57647200	1.40181700
H	1.82872600	2.85842700	1.46829900
H	2.52341300	1.49397200	2.35370700
C	2.60695000	2.09048100	-1.44405600
H	3.58638200	2.57677200	-1.40277000
H	2.52423000	1.49207100	-2.35428000
H	1.82727400	2.85646300	-1.47061300
C	3.82306500	-0.08681200	-0.00012800
H	3.79448800	-0.72423900	-0.88782100
H	4.74741300	0.49927000	-0.00102800
H	3.79553000	-0.72307500	0.88843500
Cl	0.76922900	-0.87664200	-2.27604300
Cl	0.76605300	-0.87226100	2.27801300
C	-2.11545600	1.45341800	-0.00231400
C	-2.81092000	2.62106400	-0.00146300
C	-2.20255400	3.99296700	0.00061900
H	-2.53954600	4.55752700	0.87961200
H	-1.11218100	3.98879800	0.00143300
H	-2.53834100	4.55976100	-0.87739500
C	-4.31276700	2.60751500	-0.00238500
H	-4.71033200	3.13230100	0.87660000
H	-4.70923800	3.13455000	-0.88052100
H	-4.71598300	1.59162700	-0.00395200
C	-0.68231300	1.28936200	-0.00163700
H	-2.71021200	0.54348500	-0.00359200
H	-0.14944200	2.24990500	-0.00206500

Zero-point correction= 0.348522 (Hartree/Particle)
 Thermal correction to Energy= 0.375735
 Thermal correction to Enthalpy= 0.376680
 Thermal correction to Gibbs Free Energy= 0.289441
 Sum of electronic and zero-point Energies= -2128.513708
 Sum of electronic and thermal Energies= -2128.486495
 Sum of electronic and thermal Enthalpies= -2128.485550
 Sum of electronic and thermal Free Energies= -2128.572789

DeltaG (solv) (kcal/mol) = 12.73

5ta

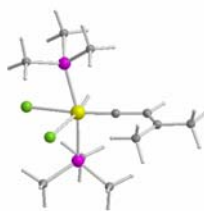


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P	-0.52444900	2.37114200	-0.13831200
P	-0.53547500	-2.36902800	-0.13893700
C	0.75693400	3.34264200	0.74698900
H	0.56342400	4.41680100	0.66797600
H	0.74679900	3.04897600	1.79957600
H	1.74317400	3.12123600	0.33203700
C	-0.51219800	3.04632700	-1.84039400
H	-1.27759200	2.51635300	-2.41271300
H	-0.71889200	4.12101400	-1.84773100
H	0.46015000	2.85491100	-2.30079000
C	-2.08956100	2.97970000	0.57953800
H	-2.14600700	2.64338000	1.61688900
H	-2.14261000	4.07138600	0.52010600
H	-2.91788600	2.52595100	0.03203300
C	0.74132600	-3.34617300	0.74674900
H	0.54284200	-4.41946100	0.66824200
H	1.72855500	-3.12950200	0.33164400
H	0.73257100	-3.05193400	1.79919100
C	-0.52543000	-3.04399100	-1.84112500
H	-0.73687500	-4.11775000	-1.84876500
H	-1.28818600	-2.51053900	-2.41373500
H	0.44798100	-2.85681500	-2.30101800
C	-2.10347200	-2.97094600	0.57821500
H	-2.92971700	-2.51407500	0.03017400
H	-2.16083900	-4.06243000	0.51907100
H	-2.15906000	-2.63419100	1.61546800
Cl	-2.52033200	0.00573000	-1.13851900
Cl	-1.36585500	0.00272200	2.21403900
C	2.80345800	-0.00742700	0.83129700
C	3.86113600	-0.00777500	-0.02025000
C	3.70883700	-0.00462000	-1.50929000
H	4.20552600	-0.88201900	-1.94217300
H	2.66192500	-0.00230100	-1.81738500
H	4.20846900	0.87278300	-1.93876900
C	5.26334700	-0.01147000	0.50734800
H	5.80938800	-0.88962500	0.14037200
H	5.81280300	0.86590400	0.14361800
H	5.29707700	-0.01353700	1.59908400
C	1.44056200	-0.00384200	0.44541300
H	2.98033800	-0.00991900	1.90774900
H	0.15046100	-0.00045100	-1.60954300

Zero-point correction= 0.347035 (Hartree/Particle)
 Thermal correction to Energy= 0.373906
 Thermal correction to Enthalpy= 0.374851
 Thermal correction to Gibbs Free Energy= 0.289217
 Sum of electronic and zero-point Energies= -2128.518668
 Sum of electronic and thermal Energies= -2128.491797
 Sum of electronic and thermal Enthalpies= -2128.490852
 Sum of electronic and thermal Free Energies= -2128.576486

DeltaG (solv) (kcal/mol) = 9.56

5tb

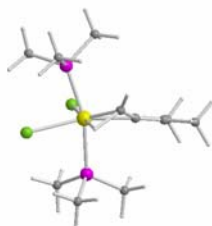


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P	-0.60409000	-2.37032500	-0.17535300
C	-1.42114400	3.03404100	-1.67227600
H	-1.61539400	4.10746900	-1.58348700
H	-0.79220700	2.84411800	-2.54545500
H	-2.36307800	2.49476900	-1.79902800
C	-1.62762800	2.97395300	1.20996300
H	-1.16347500	2.65929800	2.14697400
H	-1.72892300	4.06303800	1.17243800
H	-2.60642400	2.49517800	1.14172200
C	0.94108200	3.35393000	-0.02488900
H	1.60562800	3.13283000	-0.86364500
H	0.72625500	4.42674600	-0.00533400
H	1.44228800	3.06846900	0.90314600
C	0.93789200	-3.35487400	-0.02489700
H	0.72206000	-4.42748600	-0.00521400
H	1.60255900	-3.13448100	-0.86374300
H	1.43945500	-3.06978300	0.90305900
C	-1.42403100	-3.03274500	-1.67228600
H	-1.61929000	-4.10599300	-1.58353100
H	-2.36545600	-2.49258000	-1.79902400
H	-0.79491500	-2.84338500	-2.54545800
C	-1.63048600	-2.97252100	1.20993600
H	-2.60885900	-2.49289400	1.14165500
H	-1.73273300	-4.06151900	1.17242000
H	-1.16608500	-2.65826200	2.14695700
Cl	-2.82798200	0.00137300	-0.11006200
Cl	-0.20474000	-0.00004800	2.30895300
H	-0.68640800	0.00032600	-1.78757000
C	1.40400800	-0.00067200	-0.60915200
C	2.76175300	-0.00125900	-1.00992400
H	2.96044500	-0.00148600	-2.08198100
C	3.79474000	-0.00156900	-0.12723700
C	5.21223500	-0.00224500	-0.61104600
H	5.74752200	0.87498600	-0.22677500
H	5.74668500	-0.87996400	-0.22672100
H	5.28262800	-0.00231700	-1.70122800
C	3.58811300	-0.00127400	1.35519100
H	2.53227400	-0.00083500	1.64089300
H	4.07495900	-0.87788600	1.80125400
H	4.07561500	0.87511100	1.80098500

Zero-point correction= 0.347433 (Hartree/Particle)
 Thermal correction to Energy= 0.374051
 Thermal correction to Enthalpy= 0.374995
 Thermal correction to Gibbs Free Energy= 0.290625
 Sum of electronic and zero-point Energies= -2128.520917
 Sum of electronic and thermal Energies= -2128.494299
 Sum of electronic and thermal Enthalpies= -2128.493354
 Sum of electronic and thermal Free Energies= -2128.577724

DeltaG (solv) (kcal/mol) = 8.85

TS1

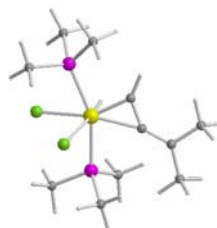


Os	0.16683800	-0.09522700	-0.20028000
P	2.43727800	0.58887100	-0.04810600
P	-1.89100200	-1.38105200	-0.12522500
C	3.36332500	0.59140800	-1.63441500
H	4.40225400	0.90342900	-1.49005500
H	3.34061000	-0.42260200	-2.04182000
H	2.88845500	1.26546200	-2.35259900
C	2.64696200	2.29098500	0.60620300
H	2.14865300	2.33696200	1.57816900
H	3.70359600	2.55174600	0.72130900
H	2.16640100	3.01176500	-0.06044200
C	3.48911400	-0.41759600	1.05475600
H	3.49964800	-1.44546100	0.68880800
H	4.50369000	-0.00842100	1.08456000
H	3.04438500	-0.41450000	2.05154100
C	-2.18172700	-2.28174800	-1.69699400
H	-3.04159400	-2.95452200	-1.62043600
H	-2.35721100	-1.56336800	-2.50265700
H	-1.28009700	-2.85467400	-1.92644400
C	-3.48610500	-0.52411300	0.17443500
H	-4.31517000	-1.23642600	0.12216000
H	-3.46362600	-0.06897900	1.16658300
H	-3.63630800	0.26598300	-0.56387800
C	-1.89045100	-2.69208700	1.14893500
H	-1.78859900	-2.22612200	2.13093000
H	-2.81410600	-3.27648500	1.09519200
H	-1.02174200	-3.33202800	0.98463500
Cl	0.28487600	-0.27557200	2.23762000
Cl	1.15799400	-2.36677900	-0.42106600
C	-1.03280300	1.63775000	-0.42056500
C	-1.92802100	2.54237000	0.00414800
C	-2.51755000	3.57011900	-0.92558100
H	-2.33510900	4.58603000	-0.54998300
H	-2.10652000	3.49656600	-1.93554700
H	-3.60863300	3.46057400	-0.99484800
C	-2.39154500	2.58478300	1.43149400
H	-2.15591600	3.55941300	1.87999400
H	-3.48277000	2.47240900	1.50310100
H	-1.90808900	1.80821800	2.02795100
C	-0.11370600	1.37382700	-1.40990800
H	0.01821000	0.08165500	-1.94153000
H	0.45201900	1.98912100	-2.10988100

Zero-point correction= 0.343986 (Hartree/Particle)
 Thermal correction to Energy= 0.370389
 Thermal correction to Enthalpy= 0.371333
 Thermal correction to Gibbs Free Energy= 0.288423
 Sum of electronic and zero-point Energies= -2128.458311
 Sum of electronic and thermal Energies= -2128.431908
 Sum of electronic and thermal Enthalpies= -2128.430964
 Sum of electronic and thermal Free Energies= -2128.513874

DeltaG (solv) (kcal/mol) = 9.39

TS2

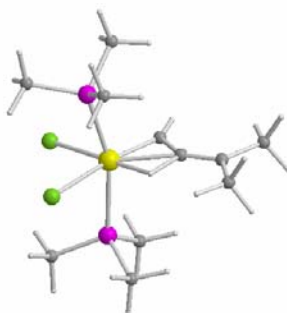


Os	-0.18683200	0.02214000	-0.16348200
P	1.74085700	-1.43153900	-0.14778500
P	-2.53297600	0.65750500	-0.09309000
C	1.42032700	-3.23571100	-0.14893200
H	2.37592500	-3.75935600	-0.03762400
H	0.76015300	-3.47957300	0.68526900
H	0.93063500	-3.54169200	-1.07331300
C	2.81654700	-1.25349800	-1.62448700
H	3.02743800	-0.20274700	-1.82226900
H	3.75046700	-1.81374200	-1.51517100
H	2.25848700	-1.65109200	-2.47672600
C	2.78122200	-1.30454300	1.36025100
H	2.26419700	-1.85946300	2.14536700
H	3.76998600	-1.74165600	1.18812300
H	2.86813000	-0.27400700	1.69807500
C	-3.38055800	0.55273300	-1.71313600
H	-4.44686600	0.77858500	-1.61623700
H	-2.91740100	1.25985300	-2.40603700
H	-3.24695600	-0.45775800	-2.10319300
C	-2.94253100	2.36592200	0.46472500
H	-4.02467500	2.45577400	0.59532200
H	-2.45329600	2.56606600	1.42169500
H	-2.62819400	3.11581400	-0.26553400
C	-3.55411300	-0.33099900	1.05835700
H	-3.12003700	-0.24961800	2.05711100
H	-4.58432300	0.03807400	1.05334100
H	-3.52322400	-1.37787700	0.75779000
Cl	-0.35397400	-0.60536200	2.26794400
Cl	-1.40507900	-2.06247300	-0.72933800
C	1.33479700	1.52909200	-0.07997500
C	2.52995700	2.16675100	-0.05748400
C	2.54189100	3.67416300	-0.17417000
H	3.10188900	3.99278000	-1.06435800
H	1.53988300	4.10245800	-0.23495600
H	3.05054400	4.12494600	0.68897800
C	3.91236900	1.59666400	0.07137600
H	4.55707300	1.98768000	-0.72760600
H	4.37377800	1.92098400	1.01502900
H	3.96208900	0.51229100	0.03611900
C	0.03953500	1.90429200	-0.17763100
H	-0.11945800	0.02804400	-1.77727800
H	-0.53801400	2.81709300	-0.21382800

Zero-point correction= 0.347569 (Hartree/Particle)
 Thermal correction to Energy= 0.372743
 Thermal correction to Enthalpy= 0.373687
 Thermal correction to Gibbs Free Energy= 0.294656
 Sum of electronic and zero-point Energies= -2128.457582
 Sum of electronic and thermal Energies= -2128.432408
 Sum of electronic and thermal Enthalpies= -2128.431464
 Sum of electronic and thermal Free Energies= -2128.510494

DeltaG (solv) (kcal/mol) = 7.85

TS3

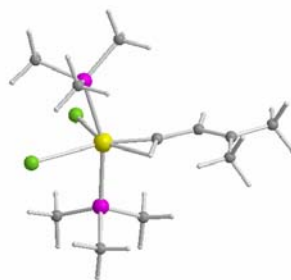


Os	-0.00760800	-0.13399500	-0.15755200
P	-2.38344000	-0.37008800	0.08889600
P	2.34672100	-0.52655900	0.09350800
C	-3.07220100	0.45898300	1.57001900
H	-4.14630200	0.27339800	1.66889700
H	-2.54590900	0.06616400	2.44351200
H	-2.89463700	1.53564800	1.50531300
C	-3.35585600	0.31145500	-1.31189300
H	-3.02679900	-0.18450300	-2.22842700
H	-4.42865600	0.14587100	-1.17198800
H	-3.16533600	1.38360700	-1.40575000
C	-2.96704700	-2.09385100	0.22209000
H	-2.49230200	-2.54903400	1.09334300
H	-4.05680200	-2.11930000	0.31921200
H	-2.64395600	-2.63893600	-0.66678800
C	3.08866400	0.28475100	1.55841200
H	4.14868200	0.03320700	1.66265200
H	2.98027900	1.36887000	1.47139100
H	2.53840800	-0.05575100	2.43906100
C	3.35681600	0.06289400	-1.32218100
H	4.41600800	-0.17723700	-1.18625600
H	2.98587000	-0.42218000	-2.22856200
H	3.24228900	1.14435900	-1.43121900
C	2.81552500	-2.28185700	0.25900800
H	2.47392500	-2.81820200	-0.62824500
H	3.89964000	-2.37570300	0.37560100
H	2.29710200	-2.69224800	1.12753400
Cl	-0.06250300	-2.12678100	-1.57487200
Cl	-0.05952500	-1.54469100	1.97954800
C	0.07277400	2.00010800	-0.32890000
C	0.12699300	3.28686100	0.07267000
C	0.17483700	4.39243600	-0.94519000
H	1.08059500	5.00035400	-0.82012900
H	0.15989000	4.01150700	-1.96878900
H	-0.67664700	5.07479800	-0.82250400
C	0.14211800	3.69985400	1.51414700
H	1.04465800	4.27969200	1.74861500
H	-0.71016200	4.35239900	1.74589800
H	0.10550200	2.84063700	2.19057000
C	0.04161200	1.19772200	-1.48007000
H	0.02275800	1.25733400	0.82807200
H	0.04998800	1.39748700	-2.55125100

Zero-point correction= 0.344107 (Hartree/Particle)
 Thermal correction to Energy= 0.370530
 Thermal correction to Enthalpy= 0.371474
 Thermal correction to Gibbs Free Energy= 0.287704
 Sum of electronic and zero-point Energies= -2128.469819
 Sum of electronic and thermal Energies= -2128.443397
 Sum of electronic and thermal Enthalpies= -2128.442453
 Sum of electronic and thermal Free Energies= -2128.526223

DeltaG (solv) (kcal/mol) = 8.91

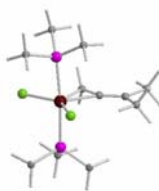
TS4



Os	0.24707100	0.00000300	0.01988900
P	0.60778900	2.36146100	0.08306100
P	0.60789400	-2.36144200	0.08305700
C	-0.57237800	3.34464000	-0.92281100
H	-0.34373900	4.41423000	-0.87941500
H	-0.50811900	2.99991300	-1.95793800
H	-1.59085900	3.17428200	-0.56539100
C	0.47506400	3.06816800	1.76960500
H	1.18529200	2.53333800	2.40534100
H	0.70117700	4.13905600	1.77750800
H	-0.53373600	2.90696200	2.15881800
C	2.24210000	2.92709600	-0.50454500
H	2.37036900	2.61244200	-1.54179100
H	2.31825700	4.01573400	-0.42111300
H	3.00992100	2.43899700	0.09894100
C	-0.57225900	-3.34468300	-0.92277000
H	-0.34356400	-4.41426100	-0.87937700
H	-1.59073600	-3.17437700	-0.56531500
H	-0.50805600	-2.99995900	-1.95790200
C	0.47525100	-3.06814800	1.76960800
H	0.70140800	-4.13902500	1.77750900
H	1.18547500	-2.53328400	2.40532100
H	-0.53354500	-2.90698100	2.15885200
C	2.24221200	-2.92700500	-0.50459700
H	3.01003000	-2.43886300	0.09885800
H	2.31842400	-4.01563800	-0.42115600
H	2.37043100	-2.61235600	-1.54185000
Cl	2.49153000	0.00004500	1.28058700
Cl	1.45109400	0.00003700	-2.05934400
C	-2.88410600	-0.00005600	-0.62576600
C	-4.07266600	-0.00007100	0.03081200
C	-4.22577300	-0.00007100	1.52192400
H	-4.79987500	-0.87791600	1.84386200
H	-3.27556800	-0.00006300	2.05848900
H	-4.79989000	0.87776600	1.84386000
C	-5.35876000	-0.00008700	-0.74152300
H	-5.96535000	-0.87819500	-0.48507600
H	-5.96537300	0.87800500	-0.48507600
H	-5.19150800	-0.00008500	-1.82095700
C	-1.55969500	-0.00003600	-0.08089800
H	-2.90121600	-0.00005600	-1.71510000
H	-1.49083400	-0.00004000	1.11141100

Zero-point correction= 0.346110 (Hartree/Particle)
 Thermal correction to Energy= 0.372503
 Thermal correction to Enthalpy= 0.373447
 Thermal correction to Gibbs Free Energy= 0.288607
 Sum of electronic and zero-point Energies= -2128.471356
 Sum of electronic and thermal Energies= -2128.444964
 Sum of electronic and thermal Enthalpies= -2128.444019
 Sum of electronic and thermal Free Energies= -2128.528860

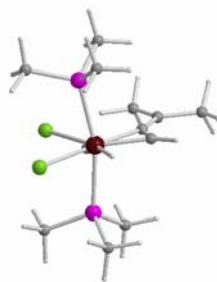
DeltaG (solv) (kcal/mol) = 10.67

3t_{Ru}

P	2.37588100	-0.47130300	0.11970900
P	-2.37585200	-0.47139200	0.11971000
C	3.30141800	-0.73621900	-1.44484000
H	4.35929600	-0.93734000	-1.24982400
H	2.85667800	-1.58250000	-1.97455400
H	3.22523700	0.15250100	-2.07727700
C	3.22367000	0.96191000	0.88834700
H	2.78970200	1.12736600	1.87703300
H	4.30134700	0.79271100	0.97706000
H	3.04234900	1.85285200	0.28206500
C	2.89573600	-1.89282700	1.15909100
H	2.50902200	-2.81332800	0.71400000
H	3.98558500	-1.95526900	1.24147300
H	2.45897200	-1.77469600	2.15405800
C	-3.30136400	-0.73662500	-1.44480000
H	-4.35924400	-0.93771300	-1.24975900
H	-3.22517900	0.15197000	-2.07741200
H	-2.85661200	-1.58300900	-1.97433800
C	-3.22372000	0.96191100	0.88809200
H	-4.30138300	0.79265300	0.97686500
H	-2.78973900	1.12759100	1.87673500
H	-3.04247800	1.85274700	0.28163100
C	-2.89564200	-1.89276200	1.15933600
H	-2.45890200	-1.77442600	2.15428900
H	-3.98548800	-1.95525400	1.24171000
H	-2.50886300	-2.81331800	0.71441600
Cl	0.00000500	0.25466300	2.32161300
Cl	0.00004200	-2.33740300	-1.35314000
C	-0.00003200	1.50912100	-0.81683100
C	-0.00008400	2.81011200	-0.53129400
C	-0.00010700	3.79766100	-1.67974200
H	0.87972900	4.45296900	-1.62890000
H	-0.00008100	3.30000100	-2.65215900
H	-0.87998900	4.45290800	-1.62891600
C	-0.00011600	3.42843800	0.83674500
H	0.87790200	4.07568200	0.96562700
H	-0.87815100	4.07566300	0.96559600
H	-0.00012000	2.67788200	1.62606400
C	0.00000500	0.58785200	-1.87833700
H	-0.90848100	0.37504600	-2.43891900
H	0.90851400	0.37509800	-2.43890100
Ru	0.00001200	-0.38075500	0.01073700

Zero-point correction= 0.349023 (Hartree/Particle)
 Thermal correction to Energy= 0.375839
 Thermal correction to Enthalpy= 0.376783
 Thermal correction to Gibbs Free Energy= 0.293146
 Sum of electronic and zero-point Energies= -2131.324485
 Sum of electronic and thermal Energies= -2131.297670
 Sum of electronic and thermal Enthalpies= -2131.296725
 Sum of electronic and thermal Free Energies= -2131.380363

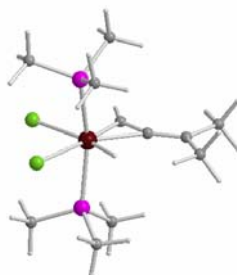
DeltaG (solv) (kcal/mol) = 8.06

3ta_{Ru}

P	2.40995600	-0.34536700	-0.14516100
P	-2.32437700	-0.66524300	-0.11689800
C	3.27475200	-0.87050800	-1.67633000
H	4.35611300	-0.94518400	-1.52420200
H	2.87933300	-1.84700100	-1.96765500
H	3.07032400	-0.15921700	-2.48086400
C	3.17043300	1.26244200	0.30051700
H	2.73791100	1.57752500	1.25360500
H	4.25669200	1.17491700	0.40057700
H	2.93326400	2.01589500	-0.45459200
C	3.04415600	-1.48915800	1.12811500
H	2.69781900	-2.49743900	0.89451300
H	4.13788700	-1.45197500	1.15964700
H	2.61780900	-1.19760800	2.08986000
C	-3.03667100	-1.58477300	-1.53369300
H	-4.08944000	-1.83263200	-1.36520100
H	-2.94437900	-0.98829200	-2.44510900
H	-2.45514800	-2.50211400	-1.65640800
C	-3.37222400	0.83534000	0.03247600
H	-4.42790200	0.56917100	0.14355700
H	-3.04620700	1.39815500	0.91050700
H	-3.24988800	1.47008400	-0.84862400
C	-2.79082000	-1.66002300	1.34092800
H	-2.44697400	-1.14388200	2.23930400
H	-3.87466000	-1.81203600	1.36860600
H	-2.26879900	-2.61665400	1.28016100
Cl	0.10583300	-0.03398900	2.19611000
Cl	0.14687300	-2.75646000	-0.10338000
C	-0.14993700	1.81587200	-0.53662500
C	-0.27880200	3.07052800	-0.04639600
C	-0.40989200	4.24115700	-0.98391700
H	0.38571200	4.97483700	-0.79705700
H	-0.36680400	3.94478500	-2.03426000
H	-1.35781300	4.76876400	-0.81197000
C	-0.30749300	3.38626500	1.41460300
H	0.50896100	4.07583400	1.67164100
H	-1.23643800	3.91337400	1.67469500
H	-0.21868300	2.48223800	2.01919700
C	-0.04742400	1.09200000	-1.66194600
H	0.01281400	1.19371900	-2.73985200
Ru	0.02650400	-0.26494000	-0.33029800
H	0.06616000	-0.90598900	-1.75886000

Zero-point correction= 0.345222 (Hartree/Particle)
 Thermal correction to Energy= 0.372276
 Thermal correction to Enthalpy= 0.373220
 Thermal correction to Gibbs Free Energy= 0.288069
 Sum of electronic and zero-point Energies= -2131.278067
 Sum of electronic and thermal Energies= -2131.251013
 Sum of electronic and thermal Enthalpies= -2131.250069
 Sum of electronic and thermal Free Energies= -2131.335219

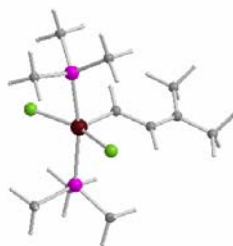
DeltaG (solv) (kcal/mol) = 1.81

3tb_{Ru}

P	2.36693500	-0.39933900	0.15420800
P	-2.36707700	-0.39864200	0.15419800
C	3.39982300	0.70667000	-0.89107100
H	3.12836600	1.74958800	-0.70798900
H	4.46478000	0.56898600	-0.67920400
H	3.21075200	0.47473900	-1.94247200
C	2.96674200	-0.07251600	1.85363900
H	2.40603000	-0.71650500	2.53513400
H	4.03849700	-0.27613400	1.94378400
H	2.77120100	0.97048400	2.11513500
C	2.97764500	-2.07202900	-0.24245800
H	4.06467200	-2.12678500	-0.12565700
H	2.48338100	-2.77981500	0.42587200
H	2.68091700	-2.31459700	-1.26496100
C	-2.97829800	-2.07118000	-0.24233000
H	-2.48437200	-2.77904700	0.42616400
H	-4.06536100	-2.12554400	-0.12567300
H	-2.68151700	-2.31398700	-1.26476000
C	-3.39960400	0.70758300	-0.89120800
H	-3.21051100	0.47554400	-1.94258100
H	-4.46461400	0.57019100	-0.67941500
H	-3.12788900	1.75043900	-0.70816100
C	-2.96681800	-0.07151000	1.85359200
H	-2.77093200	0.97143800	2.11503500
H	-4.03864300	-0.27476400	1.94373000
H	-2.40633400	-0.71565100	2.53513000
Cl	-0.00035400	-1.82060400	-1.98915400
Cl	-0.00030700	-2.03285000	1.56330400
C	0.00025600	1.10146800	-1.51343900
H	0.00027700	1.04592300	-2.59505600
C	0.00036200	1.90238900	-0.43351000
C	0.00055300	3.15806900	0.06052400
C	0.00045800	3.47387500	1.52315700
H	-0.87698100	4.07793400	1.79146800
H	0.00026700	2.56739800	2.13159600
H	0.87802100	4.07768000	1.79163500
C	0.00087800	4.33445200	-0.87885000
H	0.87987200	4.96940900	-0.70526000
H	0.00091200	4.02577900	-1.92616100
H	-0.87789100	4.96976500	-0.70542400
Ru	-0.00003800	-0.14914000	-0.09642100
H	0.00014300	0.61450800	1.28566100

Zero-point correction= 0.344989 (Hartree/Particle)
 Thermal correction to Energy= 0.371943
 Thermal correction to Enthalpy= 0.372888
 Thermal correction to Gibbs Free Energy= 0.288989
 Sum of electronic and zero-point Energies= -2131.282843
 Sum of electronic and thermal Energies= -2131.255889
 Sum of electronic and thermal Enthalpies= -2131.254944
 Sum of electronic and thermal Free Energies= -2131.338843

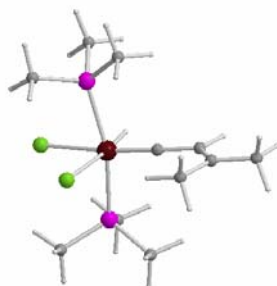
DeltaG (solv) (kcal/mol) = 1.52

3tc_{Ru}

Ru	-0.40010000	-0.35095800	0.02607000
P	-2.40934200	0.90957300	0.10717300
P	1.30665600	-2.01230300	0.01714800
C	-2.51855900	2.23323500	1.37165000
H	-3.53008100	2.64639500	1.43605900
H	-2.21570400	1.81347900	2.33362600
H	-1.81694000	3.03171500	1.11549800
C	-2.96432400	1.73045400	-1.43617300
H	-2.94903700	0.99603300	-2.24456900
H	-3.96772800	2.15264600	-1.32295000
H	-2.26622900	2.53304900	-1.68982400
C	-3.80371800	-0.21050200	0.52791200
H	-3.59784300	-0.68382200	1.49180500
H	-4.75232100	0.33285400	0.58632000
H	-3.87607900	-0.98635600	-0.23889200
C	2.56865400	-2.01178700	1.34924000
H	3.17006000	-2.92587100	1.32350500
H	3.22668000	-1.14810700	1.22332300
H	2.06119200	-1.91695600	2.31189700
C	2.29138700	-2.15762400	-1.52297000
H	2.93239400	-3.04475500	-1.51248200
H	1.59721600	-2.20053900	-2.36564300
H	2.91147700	-1.26401700	-1.63394900
C	0.51056700	-3.66116300	0.17989700
H	-0.20548200	-3.78305000	-0.63717800
H	1.24837000	-4.46919600	0.14403600
H	-0.02706700	-3.70699400	1.13097800
Cl	-1.01535100	-1.06850300	-2.21625800
Cl	-0.25231400	-0.23459500	2.44713700
C	1.82402300	1.56158500	0.21490700
C	2.65783000	2.55147200	-0.20993000
C	3.81569000	2.97760000	0.64346100
H	3.74312700	4.04571900	0.88666700
H	3.86633800	2.41532200	1.57848900
H	4.76465700	2.84969200	0.10633700
C	2.53169700	3.28378200	-1.51251700
H	2.45592800	4.36394700	-1.33472500
H	3.43628800	3.13543000	-2.11596300
H	1.67559300	2.97169400	-2.11108600
C	0.65748200	1.07960900	-0.47142300
H	2.02817300	1.10203300	1.18016500
H	0.35764300	1.61545800	-1.38262500

Zero-point correction= 0.348247 (Hartree/Particle)
 Thermal correction to Energy= 0.375686
 Thermal correction to Enthalpy= 0.376630
 Thermal correction to Gibbs Free Energy= 0.289031
 Sum of electronic and zero-point Energies= -2131.332697
 Sum of electronic and thermal Energies= -2131.305258
 Sum of electronic and thermal Enthalpies= -2131.304314
 Sum of electronic and thermal Free Energies= -2131.391914

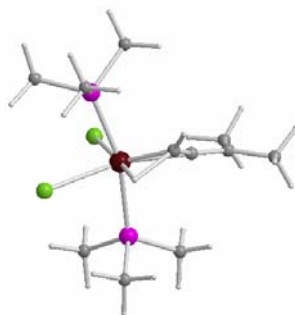
DeltaG (solv) (kcal/mol) = 6.96

5tb_{Ru}

Ru	-0.33136700	0.00030700	-0.24265500
P	-0.64955800	2.36409200	-0.20029800
P	-0.65568700	-2.36258800	-0.20034100
C	-1.45964700	3.02664100	-1.70277900
H	-1.67517900	4.09532200	-1.60449000
H	-0.81624800	2.85979200	-2.57027900
H	-2.38918500	2.47026400	-1.84596300
C	-1.69966600	2.93471000	1.17982300
H	-1.24154400	2.61211900	2.11713200
H	-1.81290900	4.02334600	1.15468600
H	-2.67038900	2.44337600	1.09164700
C	0.87334000	3.37590500	-0.01951700
H	1.55065600	3.18483300	-0.85571200
H	0.63733000	4.44402900	0.01717300
H	1.37119000	3.08471700	0.90874700
C	0.86484600	-3.37798600	-0.01978600
H	0.62645200	-4.44557700	0.01701900
H	1.54242600	-3.18844600	-0.85611700
H	1.36351800	-3.08783900	0.90836600
C	-1.46783100	-3.02290200	-1.70266000
H	-1.68627300	-4.09098700	-1.60438200
H	-2.39586300	-2.46388100	-1.84540800
H	-0.82426500	-2.85770800	-2.57034700
C	-1.70697800	-2.93082000	1.17987600
H	-2.67672500	-2.43758800	1.09165400
H	-1.82244400	-4.01922900	1.15485600
H	-1.24819500	-2.60904800	2.11714000
Cl	-2.87396900	0.00362600	-0.21849100
Cl	-0.18443800	-0.00013600	2.29145200
H	-0.67228100	0.00096200	-1.79878300
C	1.34179300	-0.00176100	-0.64295500
C	2.68949800	-0.00343200	-1.06319200
H	2.87186400	-0.00419400	-2.13825000
C	3.72957600	-0.00422800	-0.18503800
C	5.14232500	-0.00617800	-0.67969600
H	5.67962600	0.87053900	-0.29734500
H	5.67736600	-0.88400700	-0.29671700
H	5.20626000	-0.00665100	-1.77003100
C	3.53131700	-0.00330500	1.29763300
H	2.47779400	-0.00168900	1.59471700
H	4.02234700	-0.88009700	1.73861500
H	4.02497500	0.87237800	1.73788000

Zero-point correction= 0.346422 (Hartree/Particle)
 Thermal correction to Energy= 0.373176
 Thermal correction to Enthalpy= 0.374120
 Thermal correction to Gibbs Free Energy= 0.289751
 Sum of electronic and zero-point Energies= -2131.306207
 Sum of electronic and thermal Energies= -2131.279453
 Sum of electronic and thermal Enthalpies= -2131.278509
 Sum of electronic and thermal Free Energies= -2131.362878

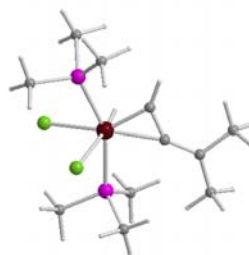
DeltaG (solv) (kcal/mol) = 1.1

TS1_{Ru}

P	2.46298300	0.56960500	-0.10260200
P	-1.86202900	-1.39046000	-0.12132200
C	3.39843700	0.52398200	-1.68270700
H	4.44263900	0.81847300	-1.53894000
H	3.35821200	-0.49793300	-2.06854800
H	2.94039700	1.19198200	-2.41743300
C	2.66655000	2.29019600	0.50503400
H	2.15526300	2.36246600	1.46869900
H	3.72197000	2.55254900	0.62840700
H	2.19802100	2.99358800	-0.18843800
C	3.50307200	-0.40687300	1.03733800
H	3.50968400	-1.44501000	0.70120800
H	4.51974400	-0.00185300	1.06351300
H	3.04813800	-0.37183600	2.02896700
C	-2.17781300	-2.34568900	-1.65684300
H	-3.03873200	-3.01247100	-1.54501000
H	-2.36074600	-1.65674200	-2.48621800
H	-1.28091400	-2.92988200	-1.87641500
C	-3.45826100	-0.52471600	0.16600700
H	-4.28706200	-1.23968500	0.16062200
H	-3.42301600	-0.02474800	1.13647200
H	-3.62689900	0.22789200	-0.60737200
C	-1.84988700	-2.65776500	1.19649800
H	-1.74228700	-2.15810500	2.16117600
H	-2.76975300	-3.25053200	1.16935000
H	-0.97692100	-3.29569000	1.04660500
Cl	0.29871700	-0.17502300	2.21889600
Cl	1.17935900	-2.39812900	-0.43324400
C	-0.99103600	1.63644500	-0.51981800
C	-1.88484600	2.53024600	-0.06368400
C	-2.63343700	3.43942800	-1.00089800
H	-2.50276200	4.48849300	-0.70456600
H	-2.30702600	3.32526500	-2.03701900
H	-3.71291500	3.24041900	-0.95790400
C	-2.19555000	2.65801500	1.39764000
H	-1.94051100	3.66663400	1.75008200
H	-3.27118600	2.53407600	1.58491400
H	-1.63532700	1.92926800	1.98723500
C	-0.11874800	1.28894800	-1.48797700
H	0.17238100	-0.17891500	-1.89826300
H	0.40636900	1.82065100	-2.27851400
Ru	0.19797200	-0.12784600	-0.24144000

Zero-point correction= 0.343138 (Hartree/Particle)
 Thermal correction to Energy= 0.369871
 Thermal correction to Enthalpy= 0.370815
 Thermal correction to Gibbs Free Energy= 0.287485
 Sum of electronic and zero-point Energies= -2131.272445
 Sum of electronic and thermal Energies= -2131.245713
 Sum of electronic and thermal Enthalpies= -2131.244768
 Sum of electronic and thermal Free Energies= -2131.328098

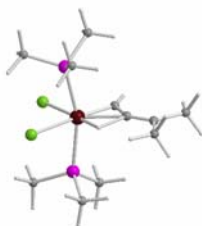
DeltaG (solv) (kcal/mol) = 2.87

TS2_{Ru}

P	1.68738500	-1.45101800	-0.10140100
P	-2.52162000	0.67808200	-0.05967900
C	1.27827700	-3.23441800	-0.00161600
H	2.19711500	-3.79831600	0.19304700
H	0.56784000	-3.37820100	0.81490100
H	0.81291800	-3.57359900	-0.92644300
C	2.79850000	-1.39811000	-1.56334300
H	3.10967700	-0.37573800	-1.78049200
H	3.67719200	-2.03696900	-1.42800300
H	2.22024300	-1.76097000	-2.41773700
C	2.72093300	-1.29301100	1.41100500
H	2.16704000	-1.78103400	2.21523500
H	3.68816600	-1.78733200	1.27265900
H	2.86079000	-0.25406100	1.70144900
C	-3.29717100	1.02004400	-1.68398000
H	-4.35929600	1.26083200	-1.57663400
H	-2.78172500	1.85193500	-2.17112300
H	-3.17903400	0.12789600	-2.30310600
C	-2.90329000	2.17485200	0.94416600
H	-3.98510300	2.26694200	1.07738800
H	-2.42961300	2.06198200	1.92318600
H	-2.54177100	3.09288900	0.47525800
C	-3.62013800	-0.54773000	0.73868700
H	-3.22376700	-0.75732900	1.73447000
H	-4.63498600	-0.14253200	0.80412200
H	-3.61108200	-1.47080100	0.16043600
Cl	-0.50937500	-0.74887100	2.19589100
Cl	-1.36317800	-1.94330100	-1.13872800
C	1.29517000	1.57415900	-0.07114200
C	2.49270000	2.21130200	-0.07876900
C	2.51453600	3.70719300	-0.28738000
H	3.05554700	3.96136400	-1.20911100
H	1.51531100	4.14099400	-0.34902500
H	3.05221200	4.20036300	0.53349500
C	3.86298300	1.62776400	0.08752600
H	4.53143000	2.00979000	-0.69510300
H	4.30222200	1.94903600	1.04265500
H	3.89245700	0.54263900	0.05582500
C	0.00642900	1.91886500	-0.18791200
H	-0.59088900	2.81998600	-0.22817100
Ru	-0.20036600	0.03316500	-0.19441800
H	-0.04340800	0.16648300	-1.76379000

Zero-point correction= 0.346236 (Hartree/Particle)
 Thermal correction to Energy= 0.371884
 Thermal correction to Enthalpy= 0.372829
 Thermal correction to Gibbs Free Energy= 0.292589
 Sum of electronic and zero-point Energies= -2131.252289
 Sum of electronic and thermal Energies= -2131.226640
 Sum of electronic and thermal Enthalpies= -2131.225696
 Sum of electronic and thermal Free Energies= -2131.305936

DeltaG (solv) (kcal/mol) = 1.9

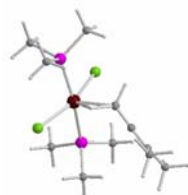
TS3_{Ru}

P	-2.36193500	-0.45413600	0.08530400
P	2.36238100	-0.45218000	0.08537900
C	-3.05061100	0.25981500	1.62485800
H	-4.11609700	0.03219600	1.72983000
H	-2.49400400	-0.16715300	2.46274300
H	-2.91018100	1.34386200	1.62245800
C	-3.38062700	0.28630900	-1.25331500
H	-3.06095500	-0.14644000	-2.20471200
H	-4.44610400	0.08574400	-1.10292800
H	-3.21985600	1.36712900	-1.28625900
C	-2.88580300	-2.20163200	0.11012000
H	-2.37595100	-2.69824100	0.93784300
H	-3.97210700	-2.27305700	0.22635700
H	-2.56217100	-2.67176900	-0.82058000
C	3.05050000	0.26295700	1.62463700
H	4.11622100	0.03644700	1.72961100
H	2.90899500	1.34686200	1.62190100
H	2.49440100	-0.16428500	2.46272000
C	3.38052200	0.28837300	-1.25359600
H	4.44611800	0.08838000	-1.10326700
H	3.06095100	-0.14487700	-2.20479900
H	3.21920600	1.36909500	-1.28689900
C	2.88760300	-2.19926100	0.11093100
H	2.56464600	-2.66996900	-0.81971600
H	3.97393000	-2.26981100	0.22750600
H	2.37788000	-2.69598500	0.93865900
Cl	0.00107900	-2.02661200	-1.75281400
Cl	0.00061800	-1.64591200	1.90970700
C	-0.00092800	1.92837300	-0.39887900
C	-0.00155800	3.20085300	0.05124600
C	-0.00212000	4.34019000	-0.93130500
H	0.87686400	4.98127000	-0.78332000
H	-0.00200500	3.99295700	-1.96661600
H	-0.88167100	4.98047800	-0.78325200
C	-0.00171800	3.57100100	1.50208400
H	0.87585700	4.18293200	1.74990400
H	-0.87981700	4.18217900	1.74990600
H	-0.00133600	2.69096600	2.15089500
C	-0.00051600	1.13781600	-1.52013100
H	-0.00056500	1.22552800	-2.60306600
Ru	0.00009600	-0.14222400	-0.15524600
H	-0.00045900	1.03227700	0.95859400

Zero-point correction= 0.343286 (Hartree/Particle)
 Thermal correction to Energy= 0.369994
 Thermal correction to Enthalpy= 0.370938
 Thermal correction to Gibbs Free Energy= 0.287177
 Sum of electronic and zero-point Energies= -2131.279860
 Sum of electronic and thermal Energies= -2131.253153
 Sum of electronic and thermal Enthalpies= -2131.252208
 Sum of electronic and thermal Free Energies= -2131.335969

DeltaG (solv) (kcal/mol) = 6.96

7ta

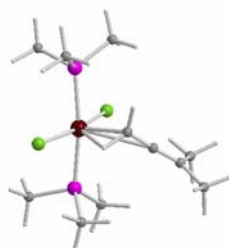


P	2.59999100	0.85786200	-0.02432300
P	-1.35093600	-1.74544500	0.14363000
C	2.98960600	1.84042700	-1.52605400
H	4.02419200	2.19734800	-1.51325800
H	2.82049400	1.21072400	-2.40280600
H	2.31961200	2.70317600	-1.58428000
C	2.99378800	2.00570400	1.35328000
H	2.79908500	1.49406000	2.29863900
H	4.03440900	2.34226900	1.31187900
H	2.33415300	2.87644500	1.29955700
C	3.96234200	-0.37373100	0.03869200
H	3.85469000	-1.05440900	-0.80987300
H	4.94414500	0.10912300	-0.00058800
H	3.88123900	-0.94889400	0.96522900
C	-2.28721200	-2.04501100	-1.40422200
H	-3.07547500	-2.79022600	-1.25933500
H	-2.72819600	-1.10629900	-1.74654300
H	-1.58565200	-2.37881800	-2.17197000
C	-2.64142200	-1.37973700	1.39364600
H	-3.40233900	-2.16583000	1.42562500
H	-2.15466100	-1.28551700	2.36706100
H	-3.11177300	-0.42343000	1.15340900
C	-0.77440300	-3.42644400	0.61795900
H	-0.27539900	-3.36320400	1.58862400
H	-1.60683400	-4.13496900	0.68063700
H	-0.05610400	-3.78248100	-0.12584800
Cl	0.57327000	-0.34205900	2.45769200
Cl	0.93586600	-0.96605400	-2.25478700
C	-1.94523800	1.69687300	-0.47834700
C	-3.14077000	2.18675900	-0.23800400
C	-3.31906500	3.42743900	0.60596400
H	-3.95810600	3.21217700	1.47113700
H	-2.36518900	3.81317500	0.96977600
H	-3.81647900	4.21489700	0.02623200
C	-4.40215000	1.57527400	-0.79734000
H	-5.08033600	1.27879400	0.01252500
H	-4.93837300	2.31155100	-1.40854100
H	-4.19933400	0.70095500	-1.41766800
C	-0.70624300	1.30684500	-0.70147800
H	-0.09517200	1.21604000	0.37269400
H	-0.17741400	1.70540900	-1.56570200
Ru	0.51927900	-0.30197300	0.03726900

Zero-point correction= 0.345273 (Hartree/Particle)
 Thermal correction to Energy= 0.372993
 Thermal correction to Enthalpy= 0.373938
 Thermal correction to Gibbs Free Energy= 0.286643
 Sum of electronic and zero-point Energies= -2131.277485
 Sum of electronic and thermal Energies= -2131.249764
 Sum of electronic and thermal Enthalpies= -2131.248819
 Sum of electronic and thermal Free Energies= -2131.336114

DeltaG (solv) (kcal/mol) = 6.47

TS5

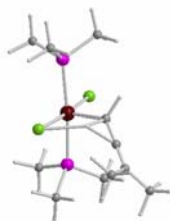


P	2.54322700	-0.71243000	0.00329500
P	-1.51617300	1.67449200	0.34247700
C	2.62960500	-2.48077700	0.49400800
H	3.66494000	-2.83042300	0.55497900
H	2.13285000	-2.59133700	1.46046100
H	2.09017400	-3.09127700	-0.23534400
C	3.48101500	-0.66952400	-1.57620900
H	3.53219200	0.36421400	-1.92452000
H	4.48797100	-1.08052900	-1.45272300
H	2.95136800	-1.25116400	-2.33602000
C	3.69316700	0.09663100	1.19055400
H	3.26653400	0.02730500	2.19490400
H	4.68039700	-0.37681200	1.18235500
H	3.79972600	1.15217600	0.92530500
C	-2.84869400	1.14548400	1.49167100
H	-3.56897000	1.95160900	1.66391100
H	-3.36958600	0.28361500	1.06835900
H	-2.39684900	0.83349600	2.43591900
C	-2.43614400	2.11292400	-1.18768300
H	-3.22948200	2.83937800	-0.98509700
H	-1.72653300	2.52872600	-1.90732500
H	-2.88110000	1.20982600	-1.61512300
C	-1.03411100	3.32213600	1.00675100
H	-0.29286000	3.75979700	0.33300900
H	-1.89681600	3.99108400	1.09301800
H	-0.58105400	3.19833900	1.99476000
Cl	1.13685200	1.94486300	-1.63499400
Cl	-0.01548100	-0.87254000	2.13785300
C	-1.44786800	-1.67370200	-1.01052000
C	-2.56614600	-2.25296900	-0.65799000
C	-3.61446700	-2.54557700	-1.70989300
H	-4.55711000	-2.04942600	-1.45099700
H	-3.30938900	-2.21589200	-2.70492000
H	-3.81309700	-3.62305500	-1.74600000
C	-2.86494500	-2.68567600	0.75508400
H	-3.82631200	-2.27050000	1.07992400
H	-2.95835400	-3.77801600	0.79021200
H	-2.08353800	-2.36648600	1.44665700
C	-0.30981000	-1.15254900	-1.45802100
H	-0.28437200	-0.08950800	-1.79598500
H	0.46116700	-1.80755300	-1.85680200
Ru	0.43521300	0.34826300	0.09148600

Zero-point correction= 0.346163 (Hartree/Particle)
 Thermal correction to Energy= 0.373332
 Thermal correction to Enthalpy= 0.374276
 Thermal correction to Gibbs Free Energy= 0.288494
 Sum of electronic and zero-point Energies= -2131.274410
 Sum of electronic and thermal Energies= -2131.247242
 Sum of electronic and thermal Enthalpies= -2131.246298
 Sum of electronic and thermal Free Energies= -2131.332079

DeltaG (solv) (kcal/mol) = 6.31

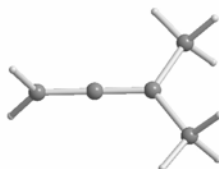
TS6



P	2.54322700	-0.71243000	0.00329500
P	-1.51617300	1.67449200	0.34247700
C	2.62960500	-2.48077700	0.49400800
H	3.66494000	-2.83042300	0.55497900
H	2.13285000	-2.59133700	1.46046100
H	2.09017400	-3.09127700	-0.23534400
C	3.48101500	-0.66952400	-1.57620900
H	3.53219200	0.36421400	-1.92452000
H	4.48797100	-1.08052900	-1.45272300
H	2.95136800	-1.25116400	-2.33602000
C	3.69316700	0.09663100	1.19055400
H	3.26653400	0.02730500	2.19490400
H	4.68039700	-0.37681200	1.18235500
H	3.79972600	1.15217600	0.92530500
C	-2.84869400	1.14548400	1.49167100
H	-3.56897000	1.95160900	1.66391100
H	-3.36958600	0.28361500	1.06835900
H	-2.39684900	0.83349600	2.43591900
C	-2.43614400	2.11292400	-1.18768300
H	-3.22948200	2.83937800	-0.98509700
H	-1.72653300	2.52872600	-1.90732500
H	-2.88110000	1.20982600	-1.61512300
C	-1.03411100	3.32213600	1.00675100
H	-0.29286000	3.75979700	0.33300900
H	-1.89681600	3.99108400	1.09301800
H	-0.58105400	3.19833900	1.99476000
Cl	1.13685200	1.94486300	-1.63499400
Cl	-0.01548100	-0.87254000	2.13785300
C	-1.44786800	-1.67370200	-1.01052000
C	-2.56614600	-2.25296900	-0.65799000
C	-3.61446700	-2.54557700	-1.70989300
H	-4.55711000	-2.04942600	-1.45099700
H	-3.30938900	-2.21589200	-2.70492000
H	-3.81309700	-3.62305500	-1.74600000
C	-2.86494500	-2.68567600	0.75508400
H	-3.82631200	-2.27050000	1.07992400
H	-2.95835400	-3.77801600	0.79021200
H	-2.08353800	-2.36648600	1.44665700
C	-0.30981000	-1.15254900	-1.45802100
H	-0.28437200	-0.08950800	-1.79598500
H	0.46116700	-1.80755300	-1.85680200
Ru	0.43521300	0.34826300	0.09148600

Zero-point correction= 0.341911 (Hartree/Particle)
 Thermal correction to Energy= 0.369473
 Thermal correction to Enthalpy= 0.370417
 Thermal correction to Gibbs Free Energy= 0.283537
 Sum of electronic and zero-point Energies= -2131.258281
 Sum of electronic and thermal Energies= -2131.230719
 Sum of electronic and thermal Enthalpies= -2131.229775
 Sum of electronic and thermal Free Energies= -2131.316655

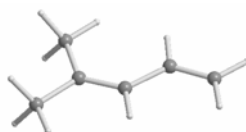
DeltaG (solv) (kcal/mol) = 5.91

alene

C	-0.93219400	-0.00013900	-0.00013100
C	-2.23959200	-0.00013200	0.00009900
H	-2.81039800	-0.00007200	-0.92688400
H	-2.81010800	-0.00023800	0.92726000
C	0.37961800	-0.00006100	-0.00036400
C	1.17089000	-1.28538600	0.00005800
H	1.82350900	-1.33714600	-0.88057900
H	1.82057200	-1.33850900	0.88281200
H	0.51960500	-2.16166200	-0.00164500
C	1.17043300	1.28561900	0.00008500
H	1.82182200	1.33839500	-0.88144800
H	0.51873700	2.16161100	0.00000000
H	1.82133500	1.33821200	0.88200000

Zero-point correction= 0.112596 (Hartree/Particle)
 Thermal correction to Energy= 0.119008
 Thermal correction to Enthalpy= 0.119952
 Thermal correction to Gibbs Free Energy= 0.083409
 Sum of electronic and zero-point Energies= -195.116850
 Sum of electronic and thermal Energies= -195.110438
 Sum of electronic and thermal Enthalpies= -195.109494
 Sum of electronic and thermal Free Energies= -195.146037

DeltaG (solv) (kcal/mol) = 4.49

bisolefine

C	1.57660300	0.30653500	-0.00014900
H	1.47389900	1.39013800	-0.00056700
C	0.36356000	-0.49111100	-0.00020800
H	0.52115500	-1.57034900	-0.00037200
C	-0.91201100	-0.05045000	-0.00012800
C	-1.31756400	1.39612800	0.00008500
H	-0.47289300	2.08655900	0.00038900
H	-1.93593000	1.62180100	-0.87839300
H	-1.93602900	1.62142800	0.87861600
C	-2.05761600	-1.02324800	0.00006400
H	-2.69850200	-0.87699800	0.87979200
H	-2.70057300	-0.87493000	-0.87777500
H	-1.71445400	-2.06112700	-0.00151300
C	2.81230300	-0.21471700	0.00019300
H	3.69649700	0.41463300	0.00014800
H	2.97518300	-1.28998100	0.00053600

Zero-point correction= 0.141681 (Hartree/Particle)
 Thermal correction to Energy= 0.149252
 Thermal correction to Enthalpy= 0.150196
 Thermal correction to Gibbs Free Energy= 0.110550
 Sum of electronic and zero-point Energies= -234.411659
 Sum of electronic and thermal Energies= -234.404089
 Sum of electronic and thermal Enthalpies= -234.403145
 Sum of electronic and thermal Free Energies= -234.442790

DeltaG (solv) (kcal/mol) = 2.58

phosphine

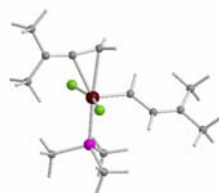


P	-0.00031900	-0.00020400	-0.60019200
C	-1.59207600	-0.38286200	0.27874200
H	-1.49093800	-0.35969400	1.36995300
H	-2.35608900	0.34193200	-0.01854500
H	-1.94472900	-1.37450100	-0.02068100
C	1.12809100	-1.18674600	0.27842400
H	2.16138000	-1.00760400	-0.03399500
H	1.07036600	-1.09898000	1.36953800
H	0.87129300	-2.21185400	-0.00554800
C	0.46447300	1.57004300	0.27819100
H	-0.21551100	2.37251000	-0.02349800
H	0.43036600	1.47145500	1.36935500
H	1.47572900	1.86718600	-0.01584500

Zero-point correction= 0.113198 (Hartree/Particle)
 Thermal correction to Energy= 0.119911
 Thermal correction to Enthalpy= 0.120855
 Thermal correction to Gibbs Free Energy= 0.083864
 Sum of electronic and zero-point Energies= -460.908207
 Sum of electronic and thermal Energies= -460.901494
 Sum of electronic and thermal Enthalpies= -460.900549
 Sum of electronic and thermal Free Energies= -460.937540

DeltaG (solv) (kcal/mol) = 3.63

7tc

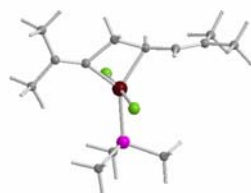


P	-0.60210100	2.00165300	-0.00395900
C	-1.75274600	2.36181400	-1.38333100
H	-2.07576900	3.40724700	-1.37024100
H	-1.23730300	2.13501600	-2.31948000
H	-2.62646100	1.71026400	-1.30125900
C	-1.49766200	2.57318100	1.49182300
H	-0.89216400	2.34561000	2.37161200
H	-1.69917200	3.64719600	1.43154100
H	-2.44684700	2.04095400	1.58607800
C	0.71513900	3.26722400	-0.20576400
H	1.27829400	3.04073600	-1.11446600
H	0.28312400	4.27045000	-0.27924700
H	1.39112000	3.23496200	0.65299700
Cl	0.38737400	-0.21017400	2.36298800
Cl	0.97147800	0.27086500	-2.34858800
Ru	0.38485600	-0.11251700	-0.03674900
C	-1.21394500	-1.00723300	-0.35419200
H	-1.19051800	-1.77298600	-1.13717600
C	-2.45998900	-0.83882400	0.33027700
H	-2.44115100	-0.21281300	1.21954100
C	-3.63763000	-1.45181200	0.01486100
C	-3.85211600	-2.34502400	-1.16894400
H	-2.95506700	-2.50901500	-1.76588400
H	-4.23732000	-3.31885600	-0.84230200
H	-4.61907000	-1.91660600	-1.82668000
C	-4.84613700	-1.24586900	0.87796800
H	-5.67491900	-0.82369600	0.29486400
H	-5.20512800	-2.20655400	1.26932500
H	-4.64312000	-0.58594200	1.72426500
C	2.26121500	-1.53750200	0.00867300
C	1.22613300	-2.35961900	-0.19959400
H	0.95203200	-2.64603700	-1.21288500
H	0.75224700	-2.87437000	0.63311400
C	3.43738500	-0.98568400	0.20180300
C	4.67852400	-1.84501900	0.21386700
H	5.37737500	-1.51302300	-0.56384000
H	5.19463600	-1.75465200	1.17748800
H	4.44687000	-2.89793800	0.04267800
C	3.63690100	0.49134900	0.40290300
H	4.16143900	0.92784200	-0.45486700
H	2.69449600	1.03060600	0.53404500
H	4.23930300	0.67391600	1.30023100

Zero-point correction= 0.347094 (Hartree/Particle)
 Thermal correction to Energy= 0.374332
 Thermal correction to Enthalpy= 0.375276
 Thermal correction to Gibbs Free Energy= 0.287759
 Sum of electronic and zero-point Energies= -1865.508279
 Sum of electronic and thermal Energies= -1865.481041
 Sum of electronic and thermal Enthalpies= -1865.480096
 Sum of electronic and thermal Free Energies= -1865.567613

DeltaG (solv) (kcal/mol) = 3.43

7td

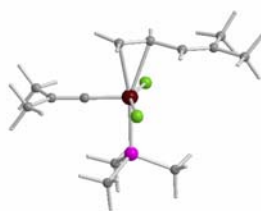


P	-0.89228300	2.24078400	-0.02679200
C	-1.43824800	3.06784900	1.50723100
H	-1.69445100	4.11247000	1.30306200
H	-2.30368900	2.54006400	1.91208000
H	-0.64397100	3.00887000	2.25307800
C	0.49127700	3.26243300	-0.65688300
H	0.80288800	2.85532500	-1.62149000
H	0.18151300	4.30646200	-0.76712800
H	1.33208100	3.21055200	0.03977100
C	-2.25671600	2.49764200	-1.21887200
H	-3.15335800	1.98179100	-0.86660900
H	-2.47478300	3.56504600	-1.32579700
H	-1.95613100	2.06814500	-2.17695600
Cl	0.04424700	0.11936400	-2.37429400
Cl	-0.52698500	0.03188800	2.43647300
Ru	-0.21854500	-0.01940600	0.02784400
C	1.40915100	-1.16506000	0.44802200
H	1.58019200	-1.20275100	1.52218900
C	2.57642600	-0.95949800	-0.39278300
H	2.42477600	-1.10324000	-1.46028000
C	3.79878700	-0.56316700	0.03625100
C	4.15519100	-0.27270400	1.46522000
H	3.31844500	-0.37295600	2.15760600
H	4.96191600	-0.93729900	1.80046700
H	4.54384800	0.74959900	1.55645600
C	4.91822000	-0.37884500	-0.94724600
H	5.29299300	0.65290100	-0.92279800
H	5.77115600	-1.02164000	-0.69271900
H	4.60830000	-0.60581300	-1.96994500
C	-1.16751500	-1.66069700	-0.04593000
C	0.32377100	-2.18389600	-0.00741100
H	0.28743700	-2.92254400	0.79837700
H	0.57889600	-2.60338400	-0.98216800
C	-2.31238600	-2.32911700	-0.10983500
C	-2.38327400	-3.83195400	-0.19023500
H	-2.97435700	-4.23490600	0.64226300
H	-2.88010000	-4.14752300	-1.11671800
H	-1.39833600	-4.30437400	-0.16494500
C	-3.62729600	-1.59697700	-0.12443000
H	-4.28017700	-1.96107600	0.67884100
H	-3.48425900	-0.52360100	0.01641700
H	-4.15837500	-1.75535000	-1.07195200

Zero-point correction= 0.350123 (Hartree/Particle)
 Thermal correction to Energy= 0.376055
 Thermal correction to Enthalpy= 0.376999
 Thermal correction to Gibbs Free Energy= 0.293916
 Sum of electronic and zero-point Energies= -1865.518585
 Sum of electronic and thermal Energies= -1865.492653
 Sum of electronic and thermal Enthalpies= -1865.491709
 Sum of electronic and thermal Free Energies= -1865.574792

DeltaG (solv) (kcal/mol) = 5.37

7te

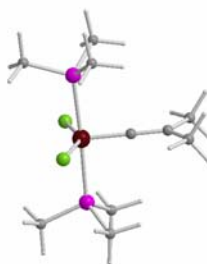


Os	-0.00760800	-0.13399500	-0.15755200
P	-2.38344000	-0.37008800	0.08889600
P	2.34672100	-0.52655900	0.09350800
C	-3.07220100	0.45898300	1.57001900
H	-4.14630200	0.27339800	1.66889700
H	-2.54590900	0.06616400	2.44351200
H	-2.89463700	1.53564800	1.50531300
C	-3.35585600	0.31145500	-1.31189300
H	-3.02679900	-0.18450300	-2.22842700
H	-4.42865600	0.14587100	-1.17198800
H	-3.16533600	1.38360700	-1.40575000
C	-2.96704700	-2.09385100	0.22209000
H	-2.49230200	-2.54903400	1.09334300
H	-4.05680200	-2.11930000	0.31921200
H	-2.64395600	-2.63893600	-0.66678800
C	3.08866400	0.28475100	1.55841200
H	4.14868200	0.03320700	1.66265200
H	2.98027900	1.36887000	1.47139100
H	2.53840800	-0.05575100	2.43906100
C	3.35681600	0.06289400	-1.32218100
H	4.41600800	-0.17723700	-1.18625600
H	2.98587000	-0.42218000	-2.22856200
H	3.24228900	1.14435900	-1.43121900
C	2.81552500	-2.28185700	0.25900800
H	2.47392500	-2.81820200	-0.62824500
H	3.89964000	-2.37570300	0.37560100
H	2.29710200	-2.69224800	1.12753400
Cl	-0.06250300	-2.12678100	-1.57487200
Cl	-0.05952500	-1.54469100	1.97954800
C	0.07277400	2.00010800	-0.32890000
C	0.12699300	3.28686100	0.07267000
C	0.14211800	3.69985400	1.51414700
H	1.04465800	4.27969200	1.74861500
H	-0.71016200	4.35239900	1.74589800
H	0.10550200	2.84063700	2.19057000
C	0.04161200	1.19772200	-1.48007000
H	0.02275800	1.25733400	0.82807200
H	0.04998800	1.39748700	-2.55125100
Si	0.18872567	4.71337409	-1.24066525
C	0.12411828	3.95336796	-3.02442997
H	1.10257819	3.62656390	-3.30853434
H	-0.54676858	3.11985790	-3.03290402
H	-0.21908875	4.69450367	-3.71568014
C	-1.32958610	5.89366793	-0.98525220
H	-1.29630127	6.30949927	0.00007842
H	-1.29319033	6.68287938	-1.70686195
H	-2.23668577	5.33961164	-1.10810097
C	1.83337746	5.71959882	-1.02564834
H	2.03985963	5.84707323	0.01647228
H	2.63955472	5.18806574	-1.48657221
H	1.72781940	6.67863693	-1.48825337

Zero-point correction= 0.349310 (Hartree/Particle)
 Thermal correction to Energy= 0.375962
 Thermal correction to Enthalpy= 0.376906
 Thermal correction to Gibbs Free Energy= 0.291370
 Sum of electronic and zero-point Energies= -1865.535411
 Sum of electronic and thermal Energies= -1865.508758
 Sum of electronic and thermal Enthalpies= -1865.507814
 Sum of electronic and thermal Free Energies= -1865.593350

DeltaG (solv) (kcal/mol) = 9.12

9t

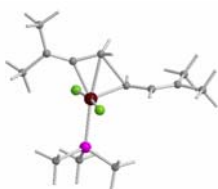


P	2.37920300	-0.42689700	0.00013100
C	3.19458000	0.35155400	1.44493900
H	4.28009300	0.21534800	1.41696100
H	2.96322300	1.41965300	1.45009300
H	2.78334700	-0.09165400	2.35480100
C	3.02572400	-2.14550000	0.00069400
H	2.65364500	-2.66341300	-0.88732600
H	4.12024500	-2.16387600	0.00027700
H	2.65437600	-2.66265800	0.88946100
C	3.19390700	0.35022900	-1.44576800
H	2.96201400	1.41820200	-1.45215700
H	4.27949400	0.21459200	-1.41784300
H	2.78274600	-0.09432400	-2.35500800
Cl	0.00004300	-0.99234300	-2.30770100
Cl	-0.00003100	-0.98766300	2.30958800
Ru	0.00001400	-0.37566000	0.00036900
C	-0.00002800	1.40798100	-0.00121700
C	-0.00011800	2.72960600	-0.00165000
C	-0.00027700	3.50244700	-1.30019100
H	-0.88294000	4.15216100	-1.36542400
H	0.88243000	4.15207100	-1.36568300
H	-0.00044200	2.83791700	-2.16735500
C	-0.00004400	3.50295600	1.29661500
H	-0.88276100	4.15260000	1.36180400
H	0.00008000	2.83875000	2.16402400
H	0.88262000	4.15269000	1.36162900
P	-2.37919400	-0.42697700	0.00011300
C	-3.19459200	0.35154200	1.44486200
H	-2.96280400	1.41954500	1.45026100
H	-4.28015700	0.21578100	1.41663800
H	-2.78372200	-0.09200600	2.35472100
C	-3.19400400	0.34982000	-1.44588600
H	-4.27961200	0.21439900	-1.41775500
H	-2.96190200	1.41774700	-1.45264200
H	-2.78305500	-0.09508600	-2.35504900
C	-3.02533000	-2.14571900	0.00096400
H	-4.11984800	-2.16440400	0.00055600
H	-2.65311400	-2.66368200	-0.88697100
H	-2.65382700	-2.66260300	0.88982600

Zero-point correction= 0.320367 (Hartree/Particle)
 Thermal correction to Energy= 0.346436
 Thermal correction to Enthalpy= 0.347380
 Thermal correction to Gibbs Free Energy= 0.264005
 Sum of electronic and zero-point Energies= -2092.058837
 Sum of electronic and thermal Energies= -2092.032769
 Sum of electronic and thermal Enthalpies= -2092.031825
 Sum of electronic and thermal Free Energies= -2092.115199

DeltaG (solv) (kcal/mol) = 8.73

3b-alba-ts1

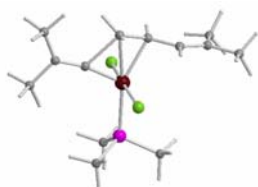


P	-0.42563400	2.35909000	0.04123400
C	-0.57264700	3.20541600	1.65610900
H	-0.62448900	4.29088900	1.52474500
H	-1.46233000	2.84024600	2.17224100
H	0.28875400	2.94542800	2.27515500
C	1.03291100	3.13120600	-0.75467500
H	1.14114400	2.69925400	-1.75198300
H	0.91458300	4.21745300	-0.81947900
H	1.92877400	2.90042000	-0.17262900
C	-1.84983300	2.96930000	-0.94075700
H	-2.78392500	2.63045400	-0.48494500
H	-1.85345600	4.06266200	-0.99036100
H	-1.77423900	2.54844900	-1.94646700
Cl	-0.00257900	0.17090500	-2.41352000
Cl	-0.91839100	-0.08237800	2.34631700
Ru	-0.32912900	-0.03282800	-0.01426600
C	2.54823800	-0.72556300	-0.33125600
H	2.41403800	-0.49106900	-1.38445900
C	3.80698800	-0.96230000	0.12782900
C	4.16781900	-1.28281700	1.54751900
H	3.31065900	-1.35880400	2.21660000
H	4.72238400	-2.22843800	1.58859000
H	4.84223500	-0.51480300	1.94666300
C	4.96938900	-0.89446300	-0.81829400
H	5.69128400	-0.13478600	-0.49177700
H	5.51193500	-1.84852700	-0.82961100
H	4.65705300	-0.66043900	-1.83818600
C	-1.31618000	-1.83119300	-0.15129600
C	0.00854700	-2.27232000	-0.24044600
H	0.41518200	-2.84789700	0.59122100
H	0.46386500	-2.42487200	-1.21675000
C	-2.60842700	-2.12817400	-0.15416200
C	-3.06889500	-3.53815200	-0.42647300
H	-3.68803700	-3.90272600	0.40316300
H	-3.68933000	-3.57695200	-1.33091000
H	-2.22959000	-4.22413300	-0.55997900
C	-3.68172600	-1.09860500	0.06265600
H	-4.41300700	-1.46139100	0.79457700
H	-3.26746900	-0.16302600	0.44616300
H	-4.22664600	-0.89482800	-0.86800700
C	1.36011700	-0.71290800	0.48108100
H	1.45549800	-1.00600500	1.53107400

Zero-point correction= 0.347995 (Hartree/Particle)
 Thermal correction to Energy= 0.373878
 Thermal correction to Enthalpy= 0.374823
 Thermal correction to Gibbs Free Energy= 0.291640
 Sum of electronic and zero-point Energies= -1865.504103
 Sum of electronic and thermal Energies= -1865.478219
 Sum of electronic and thermal Enthalpies= -1865.477275
 Sum of electronic and thermal Free Energies= -1865.560458

DeltaG (solv) (kcal/mol) = 4.7

3b-alba-ts2



P	-0.81601000	2.18915900	-0.03630600
C	-1.39485100	2.99958800	1.49751500
H	-1.64941400	4.04704500	1.30736400
H	-2.26992800	2.46772900	1.87700400
H	-0.61587200	2.92743900	2.25834000
C	0.56746100	3.24493500	-0.62083500
H	0.90669200	2.86083300	-1.58579400
H	0.24827000	4.28680600	-0.72533300
H	1.39398000	3.19471800	0.09299300
C	-2.15107000	2.49839900	-1.25135400
H	-3.07506400	2.02480200	-0.91128600
H	-2.32116300	3.57304600	-1.37068900
H	-1.85623300	2.04828800	-2.20172500
Cl	0.03419100	0.03571400	-2.37784000
Cl	-0.12912900	0.05943900	2.47031400
Ru	-0.12371700	-0.08297500	0.04638000
C	1.40679000	-1.55469900	0.37723500
H	1.58202500	-1.59629000	1.44892400
C	2.51748200	-1.17110400	-0.47468600
H	2.37564000	-1.30894300	-1.54379800
C	3.68320400	-0.63292100	-0.03761600
C	3.99959000	-0.33776700	1.40026100
H	3.13099800	-0.38761100	2.05889900
H	4.76160400	-1.03380900	1.77556400
H	4.43083000	0.66636700	1.49188800
C	4.77202000	-0.30298800	-1.01614000
H	5.01805400	0.76627000	-0.97923900
H	5.69635700	-0.83958800	-0.76453100
H	4.49474400	-0.55599000	-2.04203700
C	-1.45493400	-1.33184700	0.00228100
C	0.26206900	-2.29539200	-0.09402200
H	-0.13882800	-2.98889800	0.64154000
H	0.25630200	-2.61732800	-1.13277300
C	-2.59113100	-2.00876300	-0.03761300
C	-2.74624000	-3.49949000	-0.17310100
H	-3.26475500	-3.91236500	0.70151700
H	-3.36002800	-3.73467400	-1.05144000
H	-1.79667800	-4.02444000	-0.28500600
C	-3.87371300	-1.21164000	0.04105600
H	-3.68023600	-0.14958900	0.20054600
H	-4.45834000	-1.32457500	-0.88043500
H	-4.49138800	-1.57122200	0.87342700

Zero-point correction= 0.349427 (Hartree/Particle)
 Thermal correction to Energy= 0.375075
 Thermal correction to Enthalpy= 0.376019
 Thermal correction to Gibbs Free Energy= 0.293328
 Sum of electronic and zero-point Energies= -1865.513199
 Sum of electronic and thermal Energies= -1865.487551
 Sum of electronic and thermal Enthalpies= -1865.486607
 Sum of electronic and thermal Free Energies= -1865.569298

DeltaG (solv) (kcal/mol) = 6.07