SUPPORTING INFORMATION FOR

Carbene Rotamer Switching Explains the Reverse Trans Effect in Forming the Grubbs Second-Generation Olefin Metathesis Catalyst

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Additional details of calculations

All energetic results are calculated with the M06-L density functional[1] and TZQS basis set at geometries optimized by M06-L with the DZQS basis set for **1** and **2** and optimized with the BP86 density functional[2,3] with the double-numerical-plus-d (DND)[4] basis set for **1m** and **2m** except for the cis–trans comparison of **C** and **D** structures, which was carried out with BP86/DND. The TZQS basis set differs from the TZQ basis set used in our previous studies[5,6] in that it uses the MG3S basis set[7] for main-group elements. We found that the TZQS and DND basis sets give similar results. The DND calculations were performed with the *DMol*^{3} program package,[4] and the DZQS and TZQS calculations were carried out with the *Gaussian 09* code.[8]

Several calculations were also carried out with the M06 functional,[9] which is a hybrid meta-GGA; M06 gave similar results to M06-L, which is a meta-GGA. We chose to employ M06-L for the full set of calcuations because it is more economical to optimize large structures with a meta-GGA. Calculations employing the *Jaguar* code with M06-L/LACV3P**++(2f) and B3LYP/ LACV3P**++(2f) energies at BP86/DND optimized structures of the truncated Grubbs-type catalysts also clearly show the carbene rotamer effect. The LACV3P basis set is a triple-zeta contraction of the LACVP basis set developed and tested at Schrödinger, Inc.

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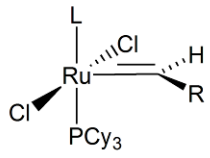
A note on nomenclature: H_2IMes and SIMes

In the literature, the 1,3-bis(mesityl)imidazolidin-2-ylidene ligand, where mesityl is 2,4,6-trimethylphenyl, is abbreviated both as H_2IMes and as SIMes, where the "S" denotes "saturated," that is, 4,5-dihydro saturation of the imidazole ring system. Here we use the former notation. Note that the 1,3-bis(mesityl)imidazolidin-2-ylidene ligand may also be called 1,3-bis(mesityl)-4,5-dihydroimidazol-2-ylidene.

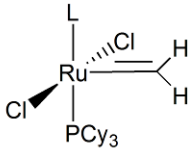
Definition of the structures in active and inactive conformations. We define the structures in active and inactive conformations of the norbornene–carbene intermediates, cis/trans isomer, and transition state structure **TS-CD** between stages **C** and **D**, as illustrated in Scheme S1.

stage **A**
active carbene



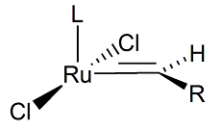
1Aa, L = PCy_3, R = Ph
2Aa, L = H_2IMes, R = Ph
1mAa, L = PCy_3, R = H
2mAa, L = H_2IMes, R = H
PMe_3-**1mAa,** L = PMe_3, R = H

stage **A**
inactive carbene



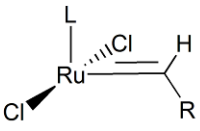
1Ai, L = PCy_3, R = Ph
2Ai, L = H_2IMes, R = Ph
1mAi, L = PCy_3, R = H
2mAi, L = H_2IMes, R = H
PMe_3-**1mAi,** L = PMe_3, R = H

stage **B**
active carbene



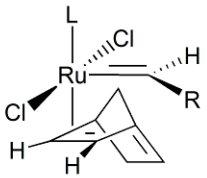
1Ba, L = PCy_3, R = Ph
2Ba, L = H_2IMes, R = Ph
1mBa, L = PCy_3, R = H
2mBa, L = H_2IMes, R = H
PMe_3-**1mBa,** L = PMe_3, R = H

stage **B**
inactive carbene

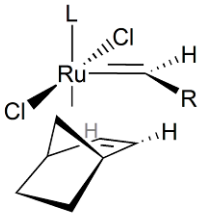


1Bi, L = PCy_3, R = Ph
2Bi, L = H_2IMes, R = Ph
1mBi, L = PCy_3, R = H
2mBi, L = H_2IMes, R = H
PMe_3-**1mBi,** L = PMe_3, R = H

stage **C**
active carbene

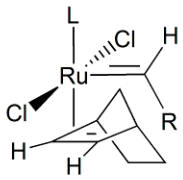


trans-**1Ca,** L = PCy_3, R = Ph
trans-**2Ca,** L = H_2IMes, R = Ph
1mCa, L = PCy_3, R = H
2mCa, L = H_2IMes, R = H



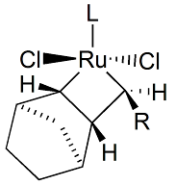
cis-**1Ca,** L = PCy_3, R = Ph
cis-**2Ca,** L = H_2IMes, R = Ph
1mCa, L = PCy_3, R = H
2mCa, L = H_2IMes, R = H

stage **C**
inactive carbene

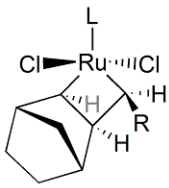


1Ci, L = PCy_3, R = Ph
2Ci, L = H_2IMes, R = Ph
1mCi, L = PCy_3, R = H
2mCi, L = H_2IMes, R = H

stage **D**

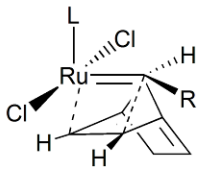


trans-**1D,** L = PCy_3, R = Ph
trans-**2D,** L = H_2IMes, R = Ph
1mD, L = PCy_3, R = H
2mD, L = H_2IMes, R = H



cis-**1D,** L = PCy_3, R = Ph
cis-**2D,** L = H_2IMes, R = Ph
1mD, L = PCy_3, R = H
2mD, L = H_2IMes, R = H

stage **TS-CD**



1mTS-CD, L = PCy_3, R = H
2mTS-CD, L = H_2IMes, R = H

Scheme S1. Structures.

Table S1. Energies (kcal/mol) of the intermediates in active/inactive carbene orientations evaluated by the BP86/DND, B3LY/LACV3P**++, and M06L/LACV3P**++ methods for **1m** and **2m**

Compound	BP86/DND	B3LYP/LACV3P++**	M06-L/ LACV3P ++**
1mAa	0	0	0
1mAi	3.3	4.1	3.3
1mBa	30.5	32.0	49.0
1mBi	19.2	21.5	35.9
2mAa	0	0	0
2mAi	7.9	8.7	7.7
2mBa	25.4	27.4	44.6
2mBi	20.6	23.3	39.8

These calculations employ with M06-L/LACV3P**++(2f) and B3LYP/ LACV3P**++(2f) energies at BP86/DND optimized structures of the truncated Grubbs-type catalysts **1m** and **2m**, and they clearly show the carbene rotamer effect.

Table S2. DFT relative energies (kcal/mol relative to **B**) of lowest-energy rotamers of **1m** and **2m** (all calculations in this table are at BP86/DND geometries).

	BP86/DND	BP86/TZQS	M06-L/TZQS	M06/TZQS
1mA	-19.2	-18.8	-34.4	-36.2
1mB	0	0.0	0.0	0.0
1mC	-1.7	-4.0	-14.0	-14.6
1mTS-CD	0.8	0.1	-7.6	-10.8
1mD	-10.4	-12.0	-21.1	-24.2
2mA	-20.6	-22.6	-39.2	-41.2
2mB	0	0.0	0.0	0.0
2mC	-3.8	-6.0	-13.7	-17.2
2mTS-CD	-3.1	-5.7	-11.8	-15.8
2mD	-16.5	-20.3	-27.6	-31.0

Rotation of carbene rotamer in the 14-electron ruthenacarbene. Figure S1 illustrates the barriers for the rotation of carbene rotamer of **1mB** and **2mB**; **a** denotes the active carbene orientation in which dihedral angle τ corresponding to L–Ru–C_α–H_1) is about 90°, while **b** indicates the inactive orientation where τ is about 180° (in this figure the inactive rotamer is taken as the reference state at zero energy). These calculations shown are carried out with the BP86/DND method and clearly show the rotation of the carbene rotamer in the 14-electron ruthenacarbene for **1m** and **2m**.

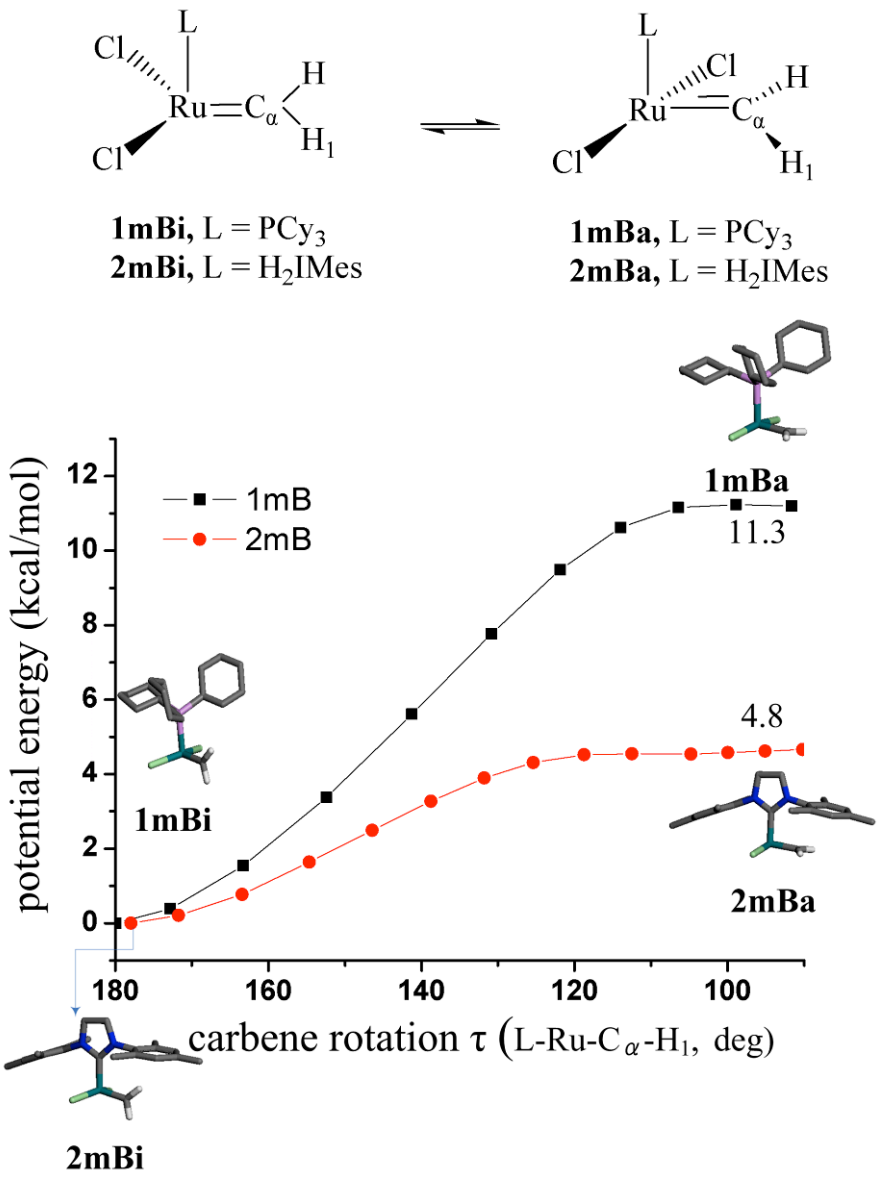
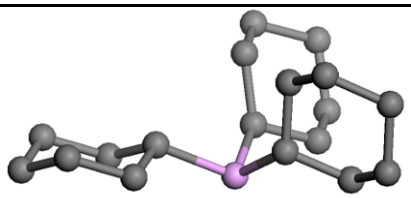


Figure S1. The potential energy as a function of carbene rotation in the 14-electron ruthenacarbene.

Structures for 1m and 2m by BP86/DND

Cartesian coordinates in angstroms and energies in hartrees

PCy_3

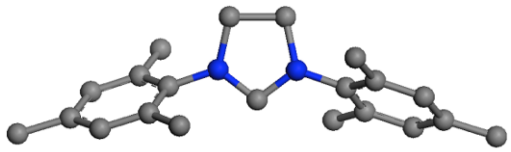


Energy: -1047.258528

P	0.52915500	-0.18508000	3.47455900
C	-0.85267000	0.41789200	4.62901900
C	0.60943100	-2.02861000	3.90283900
C	2.20290700	0.44080600	4.11147500
C	2.44649800	1.90553800	3.69121400
C	3.90716400	2.32062500	3.92375500
C	4.33876700	2.08519100	5.37684900
C	4.08380800	0.63579000	5.80878800
C	2.61950500	0.22540900	5.57665800
C	-1.08459000	1.93407400	4.47255600
C	-2.39143000	2.37773600	5.14623900
C	-2.43043000	1.96793100	6.62366600
C	-2.18341000	0.46380400	6.79082800
C	-0.87202000	0.02485600	6.11729800
C	-0.72975000	-2.70518000	3.54178500
C	-0.69627000	-4.22560000	3.76050500
C	0.45683200	-4.88335000	2.99591500
C	1.79426400	-4.22875000	3.35662200
C	1.76346800	-2.70849000	3.13656300
H	-1.72828000	-0.06978000	4.15978400
H	0.78732300	-2.16457000	4.98345000
H	2.89133400	-0.16285000	3.49048900
H	2.17244300	2.04151100	2.63335600
H	1.78964500	2.57278500	4.27149000
H	4.04654500	3.37943800	3.65148100
H	4.55988000	1.73728500	3.25062500
H	3.77165400	2.76407700	6.03792500
H	5.40229500	2.34162200	5.50765200
H	4.34803100	0.50027500	6.87030600
H	4.74484800	-0.03743000	5.23512200
H	1.97550600	0.82893600	6.23452700
H	2.47341600	-0.82458000	5.87133700
H	-0.24541000	2.48174300	4.93167100
H	-1.09065000	2.20611500	3.40487300
H	-3.24472000	1.91777500	4.61700900
H	-2.51426000	3.46858700	5.04756100
H	-3.39492000	2.25105200	7.07568200
H	-1.65315000	2.52618900	7.17522200
H	-3.02549000	-0.09394000	6.34315000
H	-2.16502000	0.19457500	7.86009300
H	-0.73973000	-1.06097000	6.23626100
H	-0.02783000	0.50093700	6.63836900
H	-1.55173000	-2.27308000	4.13226100
H	-0.96174000	-2.49203000	2.48351100
H	-1.65924000	-4.66688000	3.45498400
H	-0.58440000	-4.43589000	4.83877500
H	0.27988400	-4.77994000	1.91104800
H	0.49082800	-5.96429000	3.20736200
H	2.61298400	-4.67332000	2.76670500
H	2.02641000	-4.43623000	4.41595500
H	1.65279900	-2.49371000	2.05894700

H	2.72998600	-2.28132000	3.44269200

H_2IMes



Energy: -925.475754

N	-0.05850846	-1.82062121	-3.43228954
C	-0.17774347	-0.55686613	-2.96053528
N	-0.55723009	0.19607755	-4.01989163
C	-0.60409949	-0.54173091	-5.32162785
C	-0.48357107	-1.99422632	-4.85706217
C	0.22114792	-2.95325888	-2.60179128
C	-0.67000442	1.62320635	-3.97528741
C	-0.68174082	-3.31738704	-1.58246118
C	-0.38493690	-4.43907864	-0.80097689
C	0.76606871	-5.20771352	-1.00458423
C	1.64675584	-4.81137879	-2.01322482
C	1.39968692	-3.69232690	-2.81789254
C	0.46794282	2.40759855	-3.68864135
C	0.32963842	3.79875641	-3.67120551
C	-0.89024140	4.43117538	-3.93459250
C	-2.00050713	3.62532693	-4.19980929
C	-1.91764193	2.22788191	-4.21928601
C	2.41061914	-3.28205671	-3.85688081
C	-1.93061989	-2.51849282	-1.32248625
C	1.04115558	-6.43160210	-0.16892081
C	-3.16029097	1.40897404	-4.45407737
C	1.80156610	1.77424643	-3.39546850
C	-1.00106479	5.93473039	-3.94014911
H	0.23972746	-0.22758003	-5.95831003
H	0.25855933	-2.56537809	-5.42894714
H	-1.08100568	-4.72165986	-0.00716319
H	2.56735550	-5.37796212	-2.17219567
H	1.20890307	4.40733335	-3.44555316
H	-2.97098673	4.09627976	-4.37657940
H	3.40138377	-3.69424981	-3.61872713
H	2.49451431	-2.18783979	-3.91741745
H	2.14335776	-3.64736348	-4.86309859
H	-2.48278956	-2.92548903	-0.46406790
H	-2.60453785	-2.52810740	-2.19526272
H	-1.67857360	-1.46512105	-1.12924255
H	0.54433836	-7.32189852	-0.59068669
H	0.67072651	-6.30882808	0.85968266
H	2.11809114	-6.64973896	-0.12087756
H	-3.16124687	0.50547802	-3.82752290
H	-3.25049234	1.08268050	-5.50450527
H	-4.05968566	1.99507272	-4.22076986
H	2.55231074	2.53901538	-3.15269717
H	2.17212849	1.19645147	-4.25862087
H	1.71562741	1.06846256	-2.55593333
H	-0.73476249	6.35195480	-4.92638497
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H	-2.02583565	6.26133446	-3.71144125
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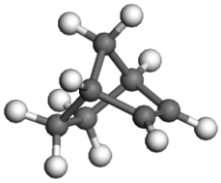
norbornene



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C	-2.66106996	0.34530369	-0.54400561
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C	0.18187020	0.41759101	-0.23984966
C	-0.71221915	1.43030756	0.45761462
C	-1.90189942	1.70578378	-0.52795152
C	-1.41043937	0.51650026	1.49028981
H	-3.68862972	0.45447607	-0.16799876
H	-2.71867753	-0.09825170	-1.54619453
H	-2.32525018	-1.43859487	0.79574190
H	-0.18461042	-1.66934573	-0.77116192
H	1.11531980	0.66004282	-0.74665176
H	-0.22309358	2.33391520	0.83828726
H	-1.54531533	2.00596959	-1.52139659
H	-2.54034634	2.51469196	-0.14280196
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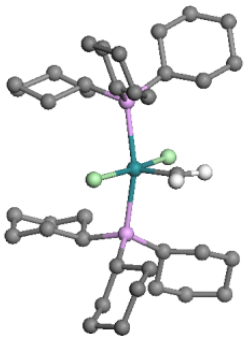
Stage A

1mA a



Energy: -7498.624958

C	0.11132200	2.10522700	1.02402100
Ru	0.11391000	0.26977000	1.00640500
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Cl	2.52825300	0.12289200	0.60591600
P	0.51302600	-0.10890000	3.42297600
C	-0.88007000	0.51014300	4.52520800
C	0.56383000	-1.95413000	3.79983700
C	2.19565400	0.48992600	4.01347800
C	2.40683800	2.01116500	3.87764900
C	3.88616700	2.37336800	4.08906300
C	4.40417100	1.87745000	5.44479500
C	4.15065800	0.37534100	5.62020200
C	2.66919200	0.01662800	5.40312300
C	-1.09961000	2.03439500	4.45484900
C	-2.42171000	2.42639100	5.13276400
C	-2.47535000	1.94688700	6.58887400
C	-2.20434000	0.44022000	6.68472000
C	-0.88254000	0.05046100	5.99851500
C	-0.77421000	-2.66392000	3.50850800
C	-0.71990000	-4.14062000	3.93369700
C	0.44450400	-4.88403000	3.26747000
C	1.77519800	-4.16650000	3.52263500
C	1.72239300	-2.68948000	3.09552200
H	-1.74982000	0.05858600	4.01849400
H	0.74179200	-2.02281000	4.88620800
H	2.84622600	0.02989300	3.25012300
H	2.08434800	2.34884100	2.88458700
H	1.79699800	2.54558500	4.62261300
H	4.01553000	3.46529000	4.00594100
H	4.47924200	1.92174900	3.27574000
H	3.89123800	2.42505800	6.25629500
H	5.47921900	2.09765000	5.55070600
H	4.46568100	0.04723900	6.62490600
H	4.76619000	-0.18932000	4.89818700
H	2.06718000	0.49844400	6.18913200
H	2.54063500	-1.06873000	5.52540100
H	-0.26984000	2.55633000	4.95644800
H	-1.11138000	2.36489800	3.40873400
H	-3.25744000	1.98317300	4.56491200
H	-2.55144000	3.52021500	5.08561900
H	-3.45240000	2.18886800	7.03883100
H	-1.71592000	2.49014600	7.18028600
H	-3.03452000	-0.10949000	6.20750400
H	-2.17991000	0.11939400	7.73948000
H	-0.73960000	-1.03662000	6.08210000

H	-0.04720000	0.52364300	6.53796000
H	-1.60749000	-2.16451000	4.02144500
H	-1.00345000	-2.59492000	2.43415000
H	-1.67824000	-4.62940000	3.69242300
H	-0.60792000	-4.19977000	5.03148100
H	0.26651600	-4.94109000	2.18030300
H	0.49177300	-5.92374000	3.63144300
H	2.59650100	-4.67379000	2.99022100
H	2.02077100	-4.22424000	4.59848300
H	1.59543500	-2.62147000	2.00410900
H	2.68568900	-2.20790000	3.31262100
P	-0.28422000	-0.06357000	-1.41686000
C	1.10601900	0.57998900	-2.50853000
C	-0.33039000	-1.90222000	-1.82534000
C	-1.96927000	0.54012500	-1.99605000
C	-2.18787000	2.05748200	-1.83326000
C	-3.66898000	2.41599300	-2.03912000
C	-4.18345000	1.94235300	-3.40416000
C	-3.92283000	0.44479500	-3.60599000
C	-2.43998000	0.08919400	-3.39405000
C	1.31870200	2.10387300	-2.41090000
C	2.63797700	2.51439200	-3.08352000
C	2.69129700	2.06033400	-4.54804000
C	2.42814700	0.55434400	-4.67025000
C	1.10923900	0.14572400	-3.98960000
C	1.00882900	-2.61486000	-1.54672000
C	0.95400900	-4.08517000	-1.99382000
C	-0.20883000	-4.83937000	-1.33669000
C	-1.54070000	-4.11966000	-1.57912000
C	-1.48732000	-2.64933000	-1.13054000
H	1.97794000	0.12323300	-2.01021000
H	-0.50952000	-1.95373000	-2.91232000
H	-2.61781000	0.06367600	-1.24117000
H	-1.86764000	2.37935500	-0.83415000
H	-1.58031000	2.60869500	-2.56783000
H	-3.80346000	3.50577500	-1.93646000
H	-4.26025000	1.94710500	-1.23449000
H	-3.67220000	2.50706300	-4.20483000
H	-5.25946000	2.15935700	-3.50716000
H	-4.23530000	0.13271300	-4.61659000
H	-4.53666000	-0.13541000	-2.89493000
H	-1.83973000	0.58740400	-4.17105000
H	-2.30629000	-0.99326000	-3.53505000
H	0.48619300	2.63057200	-2.90292000
H	1.32953600	2.41623000	-1.35933000
H	3.47698400	2.06564500	-2.52506000
H	2.76224900	3.60799200	-3.01773000
H	3.66652300	2.31527500	-4.99490000
H	1.92821800	2.60993300	-5.12880000
H	3.26166500	0.00067200	-4.20353000
H	2.40403800	0.25175400	-5.73037000
H	0.97116400	-0.94062000	-4.09145000
H	0.27124500	0.62407300	-4.52026000
H	1.84100900	-2.10737000	-2.05357000
H	1.23985000	-2.56240000	-0.47188000
H	1.91276700	-4.57731000	-1.76135000
H	0.84023600	-4.12832000	-3.09218000
H	-0.02887000	-4.91227000	-0.25065000
H	-0.25569000	-5.87386000	-1.71539000
H	-2.36067000	-4.63482000	-1.05230000
H	-1.78858000	-4.16180000	-2.65514000
H	-1.35827000	-2.59753000	-0.03859000
H	-2.45115000	-2.16497000	-1.33838000
H	-0.81260000	2.68406300	1.18225200
H	1.03382800	2.68906600	0.87607700

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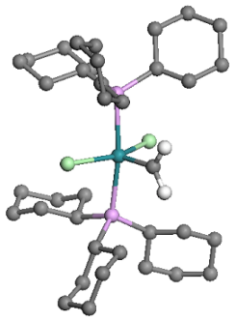

Energy: -7498.619690

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Cl	-2.18527500	-0.41910100	1.37934300
Cl	2.41810400	-0.41266000	0.62328500
P	0.52251200	-0.12908100	3.45594500
C	-0.88273700	0.50006200	4.55201800
C	0.59871100	-1.96154000	3.94122500
C	2.20885800	0.48245600	4.05141200
C	2.50999700	1.95494800	3.70320900
C	3.98373700	2.29891900	3.98181400
C	4.38896400	1.98564800	5.42731400
C	4.07261400	0.52723100	5.77938200
C	2.59430200	0.19392800	5.51665400
C	-1.15197400	2.01126700	4.40174200
C	-2.45848300	2.42053500	5.10241500
C	-2.47281800	2.00666100	6.57858900
C	-2.19566400	0.50653900	6.72658500
C	-0.87722900	0.10419900	6.04355400
C	-0.72739700	-2.71668100	3.71484100
C	-0.63875700	-4.16140200	4.23416300
C	0.52490500	-4.92803200	3.59484300
C	1.84484100	-4.17360000	3.78626100
C	1.75610900	-2.72881400	3.26854700
H	-1.73832600	-0.00496300	4.07048000
H	0.79305400	-1.96221000	5.02676600
H	2.86989100	-0.11481100	3.40027100
H	2.29411300	2.13736900	2.64281800
H	1.86475200	2.62345300	4.29703500
H	4.16376800	3.36271700	3.75443400
H	4.61842000	1.71732900	3.29084500
H	3.83866100	2.65292000	6.11540500
H	5.46132800	2.19280700	5.57872700
H	4.31459400	0.32405000	6.83601100
H	4.71069200	-0.14166200	5.17509500
H	1.97388300	0.80749000	6.18792100
H	2.40497800	-0.85616900	5.78043800
H	-0.31654800	2.58797800	4.83263700
H	-1.22065300	2.27294000	3.33832100
H	-3.30596800	1.94334000	4.58048800
H	-2.60212100	3.50978900	5.00641200
H	-3.43948200	2.26600600	7.04122800
H	-1.69927900	2.57466400	7.12678700
H	-3.02701900	-0.06353700	6.27501700
H	-2.16199800	0.22232300	7.79165400
H	-0.72146200	-0.97710700	6.16788800
H	-0.04552200	0.60531700	6.56124700
H	-1.56540400	-2.20423300	4.20703300
H	-0.97007300	-2.72356500	2.64205500
H	-1.59266900	-4.68004900	4.04274700

H	-0.50613400	-4.14752400	5.33139300
H	0.33033000	-5.05058200	2.51463300
H	0.59515500	-5.94383400	4.01833000
H	2.66779300	-4.69580200	3.27065500
H	2.10761600	-4.16270100	4.85973500
H	1.60727200	-2.73756700	2.17869000
H	2.71669100	-2.22321400	3.43505800
P	-0.29019600	-0.08494200	-1.44694600
C	1.10869600	0.56641300	-2.53807200
C	-0.36494100	-1.90858400	-1.96356000
C	-1.97974400	0.53426900	-2.02514300
C	-2.28308700	1.99889500	-1.64565500
C	-3.75939400	2.34322800	-1.90856000
C	-4.17216900	2.05811000	-3.35772800
C	-3.85262400	0.60802700	-3.74092400
C	-2.37135200	0.27539600	-3.49413800
C	1.36158200	2.07959500	-2.37720600
C	2.66242800	2.50843800	-3.07694600
C	2.67794600	2.10587500	-4.55625000
C	2.41700800	0.60394700	-4.71508300
C	1.10433400	0.18206500	-4.03253400
C	0.96506500	-2.66434800	-1.76300800
C	0.87615800	-4.09730400	-2.31374200
C	-0.28054100	-4.88117600	-1.68315000
C	-1.60421700	-4.12606500	-1.84423900
C	-1.51461000	-2.69227000	-1.29693700
H	1.96979300	0.06637000	-2.06106100
H	-0.56849400	-1.88972500	-3.04732800
H	-2.63700400	-0.07728500	-1.38366000
H	-2.06142200	2.16112300	-0.58323700
H	-1.64355000	2.68066000	-2.23037100
H	-3.94221100	3.40135400	-1.65832400
H	-4.38815000	1.74533500	-1.22615200
H	-3.62819600	2.74088600	-4.03561000
H	-5.24611300	2.26441000	-3.49870800
H	-4.10127200	0.42416400	-4.79951000
H	-4.48377300	-0.07458600	-3.14476300
H	-1.75665800	0.90528500	-4.15575400
H	-2.17924600	-0.76819100	-3.78103000
H	0.51942900	2.64992900	-2.80327900
H	1.42845800	2.33500600	-1.31215700
H	3.51609400	2.03666300	-2.56020500
H	2.79431700	3.59851800	-2.97328100
H	3.64071500	2.37945400	-5.01869600
H	1.89679000	2.66936700	-5.09822300
H	3.25533000	0.03958900	-4.26927200
H	2.38413700	0.32742900	-5.78218400
H	0.96016200	-0.89980300	-4.16503200
H	0.26601800	0.67809800	-4.54459500
H	1.79832700	-2.13927000	-2.24987500
H	1.21552800	-2.69358900	-0.69231800
H	1.83259400	-4.61752000	-2.14016400
H	0.73647000	-4.05889100	-3.40949100
H	-0.07567000	-5.02881000	-0.60799800
H	-0.35292100	-5.88688000	-2.12965000
H	-2.42046800	-4.66143900	-1.33151900
H	-1.87825300	-4.09303900	-2.91447800
H	-1.35737200	-2.72327700	-0.20869900
H	-2.47779300	-2.18610200	-1.44572200
H	0.30922300	2.57392200	1.92932500
H	-0.07219900	2.59010100	0.12835200

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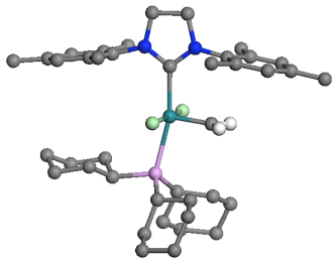

Energy: -7376.889236

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Cl	-2.48578370	-0.19647906	-0.36668323
P	0.10289844	0.40685231	1.84885077
C	-1.47130188	0.97118052	2.71568234
C	0.41038550	-1.28705965	2.60942951
C	1.59452503	1.40731563	2.41802038
C	1.48947621	2.90921170	2.09313556
C	2.84741286	3.60270213	2.28560481
C	3.38845078	3.39857690	3.70554079
C	3.44597477	1.91039939	4.06888126
C	2.08635378	1.21800187	3.86689108
C	-2.01450923	2.32793010	2.22925361
C	-3.42824163	2.57303114	2.77790226
C	-3.47027068	2.49550883	4.30833787
C	-2.88330921	1.17169056	4.81199507
C	-1.47071681	0.92394928	4.25639536
C	-0.76550373	-2.26525047	2.41848855
C	-0.49670931	-3.58890316	3.15111123
C	0.82084877	-4.23053679	2.70355501
C	1.99267952	-3.25210526	2.84139072
C	1.71786349	-1.93143613	2.10667955
H	-2.18779694	0.22045440	2.34311451
H	0.51983772	-1.11126448	3.69272788
H	2.36652382	1.00705571	1.73801839
H	1.14425874	3.05045099	1.06029956
H	0.74972895	3.38630992	2.75609317
H	2.74807142	4.67876325	2.06565719
H	3.56303983	3.19497326	1.55203945
H	2.73158037	3.92211286	4.42352445
H	4.38677323	3.85545833	3.80493513
H	3.77233180	1.78200315	5.11437041
H	4.20060702	1.40862173	3.43805617
H	1.35900576	1.64530268	4.57456083
H	2.18653792	0.15370360	4.12180560
H	-1.35297146	3.14346453	2.55972679
H	-2.04118935	2.34361124	1.13296142
H	-4.11046648	1.81863905	2.34997776
H	-3.79307600	3.555645463	3.55564546
H	-4.50525812	2.61390274	4.66884979
H	-2.89166000	3.335209047	3.33520905
H	-3.54212475	0.34060406	4.50515074
H	-2.85400155	1.15900462	5.91472096
H	-1.09837645	-0.04127628	4.62941231
H	-0.79292075	1.69839894	4.64935825
H	-1.70557641	-1.83010460	2.78362762
H	-0.91510388	-2.45810483	1.34494441
H	-1.33812402	-4.28049555	2.97993476
H	-0.46207515	-3.40059715	4.23963030
H	0.72964547	-4.53031950	1.64723670
H	1.01711729	-5.14894532	3.28208898

H	2.91826765	-3.70588781	2.45180391
H	2.17309656	-3.04188860	3.91107633
H	1.64024332	-2.12015688	1.02453229
H	2.57121667	-1.25103210	2.23218639
H	0.51890880	2.67827463	-1.13914648
H	-1.32958014	2.45626285	-0.97143497
N	-0.06317318	-1.74172721	-3.08562685
C	-0.17637230	-0.45829439	-2.66008496
N	-0.37010215	0.31794646	-3.75969346
C	-0.40093069	-0.45103757	-5.02660349
C	-0.17690130	-1.88858396	-4.55721862
C	0.15540698	-2.94909036	-2.32757461
C	-0.54917024	1.74224351	-3.84830202
C	-0.95797721	-3.73954226	-1.96198218
C	-0.71735362	-4.99699431	-1.39049343
C	0.57730193	-5.49332485	-1.19151801
C	1.65574408	-4.68423575	-1.57125484
C	1.47621841	-3.42023363	-2.15357752
C	0.57567579	2.56293517	-4.09069035
C	0.36355948	3.93615675	-4.27384443
C	-0.91731404	4.50453445	-4.23709163
C	-2.01128921	3.65445684	-4.02838367
C	-1.85881554	2.27310454	-3.84384837
C	2.67112149	-2.62858725	-2.61208879
C	-2.37096795	-3.28044326	-2.20320671
C	0.80152810	-6.85937160	-0.59184785
C	-3.06330992	1.39611617	-3.63606616
C	1.96822173	1.99661475	-4.14025818
C	-1.10929872	5.99039706	-4.40475447
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H	0.74224625	-2.33411305	-4.96235644
H	-1.57488061	-5.61727537	-1.11593873
H	2.67545559	-5.05611852	-1.44275016
H	1.22907067	4.57922661	-4.45520467
H	-3.02037047	4.07529486	-4.01518459
H	3.60010527	-3.18097645	-2.41358683
H	2.73179779	-1.65527433	-2.10253272
H	2.63353498	-2.42617333	-3.69421966
H	-3.08753442	-4.02943691	-1.84007730
H	-2.57405264	-3.12542828	-3.27454809
H	-2.57550474	-2.32884474	-1.68954718
H	-0.00578938	-7.55362168	-0.86290321
H	0.83319457	-6.81102259	0.50884827
H	1.75277485	-7.29528559	-0.92806332
H	-3.01133038	0.86617931	-2.67271748
H	-3.15126041	0.63122343	-4.42379794
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H	2.69986047	2.78735866	-4.35358642
H	2.07026742	1.23166382	-4.92570521
H	2.24021819	1.52002701	-3.18529838
H	-0.35371373	6.42080257	-5.07720499
H	-1.01753732	6.51043527	-3.43711878
H	-2.10263905	6.22717587	-4.81209823
H	-1.36763904	-0.31234805	-5.53044373
H	-1.01454424	-2.55523240	-4.80445365

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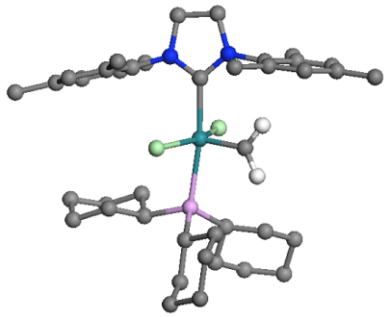


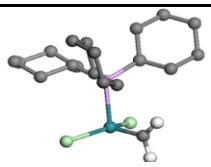
Energy: -7376.876660

C	-0.52955651	1.90249031	-0.80947210
Ru	-0.06460360	0.12816506	-0.62448503
Cl	2.33200234	0.21175711	-0.83122987
Cl	-2.19628792	-0.88043639	-0.18656825
P	0.18571127	0.33426135	1.87909687
C	-1.39248829	0.76976430	2.82506419
C	0.66602687	-1.30644908	2.68526431
C	1.61420224	1.45935706	2.41830604
C	1.34403295	2.95551189	2.15505343
C	2.62034543	3.79445405	2.33173308
C	3.23787040	3.60173670	3.72044907
C	3.48998969	2.11618303	4.00086562
C	2.20984725	1.27929498	3.83110687
C	-2.19014041	1.94463574	2.22464390
C	-3.56592182	2.08195515	2.89727005
C	-3.45316970	2.22318069	4.41927975
C	-2.64961447	1.06243461	5.01589072
C	-1.26727663	0.93161873	4.35270299
C	-0.41802797	-2.40060570	2.61340548
C	0.01367518	-3.64587065	3.40598925
C	1.35923376	-4.19671729	2.92010804
C	2.43755001	-3.10790039	2.92630845
C	1.99574772	-1.86489322	2.13790219
H	-2.00265699	-0.12582582	2.62442243
H	0.81833920	-1.07128478	3.75202613
H	2.38361740	1.15328242	1.68831249
H	0.96014875	3.10097525	1.13829638
H	0.57461514	3.32368584	2.85363866
H	2.39140586	4.85834975	2.15476829
H	3.35152023	3.49539289	1.56134033
H	2.54867280	4.00344925	4.48502864
H	4.17500501	4.17528432	3.81036796
H	3.88968727	1.97911120	5.01935937
H	4.26107014	1.74063483	3.30577919
H	1.47909564	1.59175254	4.59259550
H	2.44653877	0.22649717	4.03326105
H	-1.63315895	2.88775387	2.34927154
H	-2.33253028	1.77735430	1.14963074
H	-4.16739006	1.18830169	2.65695170
H	-4.10013934	2.94482133	2.46642600
H	-4.45495975	2.27156568	4.87680551
H	-2.94959397	3.17613716	4.66236531
H	-3.20928747	0.12114523	4.87446627
H	-2.52823912	1.19538447	6.10407757
H	-0.72667460	0.08526158	4.80102361
H	-0.68373620	1.83824855	4.57805858
H	-1.37513815	-2.03777836	3.01082519
H	-0.60563940	-2.66886954	1.56353409
H	-0.76763137	-4.41979606	3.32911814
H	0.09053729	-3.38610467	4.47736184

H	1.24285535	-4.58072950	1.89304078
H	1.67189709	-5.04994932	3.54494644
H	3.37763220	-3.49818654	2.50283125
H	2.66279662	-2.81892991	3.96869131
H	1.86751071	-2.12703759	1.07728787
H	2.79015072	-1.10709385	2.16397871
H	-0.73760216	2.35654688	-1.78225655
H	-0.62552663	2.59046592	0.03899629
N	0.02647433	-1.65127350	-3.17965713
C	-0.13621168	-0.36965303	-2.73929531
N	-0.14708104	0.41684036	-3.85163154
C	-0.03359097	-0.33720047	-5.12563600
C	0.19790842	-1.76720914	-4.64788393
C	-0.03812768	-2.88765653	-2.43988025
C	-0.41389119	1.82292977	-3.98316210
C	-1.29358274	-3.51964490	-2.29100431
C	-1.33941319	-4.76378730	-1.65411053
C	-0.18536795	-5.41084264	-1.19744493
C	1.04493687	-4.78476585	-1.41403181
C	1.15023115	-3.53550855	-2.04537162
C	0.66237677	2.71901345	-4.14344593
C	0.36887858	4.07138819	-4.35752641
C	-0.94635508	4.54832560	-4.42227760
C	-1.98837558	3.62638916	-4.27192099
C	-1.75128465	2.26297683	-4.05398727
C	2.51668206	-2.98076318	-2.35486043
C	-2.55866773	-2.93385569	-2.86191539
C	-0.27169810	-6.74088883	-0.49054646
C	-2.90563089	1.31561242	-3.85023657
C	2.09216908	2.24974125	-4.06790103
C	-1.22585699	6.01765484	-4.62011937
H	0.79873816	0.05651466	-5.72364828
H	1.20971403	-2.13160920	-4.87811531
H	-2.31046463	-5.24771121	-1.52251860
H	1.96409977	-5.28664350	-1.10075061
H	1.19853520	4.77448686	-4.46900311
H	-3.02287845	3.97765786	-4.31339882
H	3.26448968	-3.38237310	-1.65753845
H	2.55002546	-1.88781321	-2.28363164
H	2.83200044	-3.27613879	-3.37040500
H	-3.43866928	-3.40547665	-2.40647443
H	-2.61708837	-3.11031422	-3.94976422
H	-2.62890253	-1.85757609	-2.67878776
H	-1.04569705	-7.38374814	-0.93444464
H	-0.53026272	-6.60542251	0.57172469
H	0.68420490	-7.28128455	-0.53093667
H	-2.88296748	0.86846512	-2.84560897
H	-2.89211653	0.48624622	-4.57295743
H	-3.86270087	1.84127708	-3.96795600
H	2.78068480	3.10524375	-4.05126451
H	2.36131582	1.63079115	-4.93919894
H	2.26961525	1.64514345	-3.16734042
H	-0.57409196	6.45016048	-5.39332005
H	-1.04523840	6.58130170	-3.69037065
H	-2.26884238	6.19479737	-4.91528602
H	-0.95806132	-0.22076757	-5.71135062
H	-0.52732254	-2.48319742	-5.05713896

Stage B

1mB i



Energy: -6451.320356

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Cl	1.56926100	-0.65127900	1.21623600
Ru	-0.63274100	0.02871400	0.80905400
Cl	-2.86094500	-0.56487400	1.20733900
H	-0.58893600	2.30501800	1.83841600
H	-0.58099800	2.58389300	-0.00522700
P	-0.63709300	-0.36967100	-1.45122300
C	0.95479800	0.18591700	-2.29786100
C	-2.19404500	0.25977300	-2.31034600
C	-0.67954200	-2.22401700	-1.81835900
C	1.15397600	-0.25583300	-3.76378200
C	2.58674100	0.04920900	-4.23647600
C	2.92802700	1.53493400	-4.07752500
C	2.69648800	1.99935300	-2.63562400
C	1.27156900	1.68678300	-2.14802800
C	-2.37668300	-0.14089700	-3.79019200
C	-3.78962100	0.21794300	-4.28290000
C	-4.08757800	1.70950000	-4.09706600
C	-3.87041800	2.13485500	-2.64086900
C	-2.46732700	1.76590600	-2.13025200
C	0.56504600	-2.98218800	-1.31230100
C	0.53423400	-4.45589500	-1.75223200
C	-0.74705400	-5.15866800	-1.29050100
C	-1.98833200	-4.40045200	-1.77314700
C	-1.96410200	-2.92657700	-1.33264600
H	1.69730300	-0.34514800	-1.67743600
H	-2.96575800	-0.26111500	-1.71772700
H	-0.67281400	-2.27712800	-2.92052500
H	0.94981300	-1.32796500	-3.89269700
H	0.44799000	0.28430200	-4.41295500
H	2.69736200	-0.26244500	-5.28819000
H	3.29872700	-0.55785400	-3.65040500
H	2.29460900	2.13021900	-4.75963700
H	3.97212000	1.72264500	-4.37581600
H	2.88566100	3.08140300	-2.54353100
H	3.41773700	1.49780200	-1.96733000
H	0.55091200	2.28506200	-2.72935100
H	1.18122400	1.98423300	-1.09613200
H	-1.64201300	0.39372700	-4.41125700
H	-2.20077500	-1.21539800	-3.94137300
H	-4.53124200	-0.37851700	-3.72324700
H	-3.89060000	-0.06771300	-5.34289400
H	-5.11869000	1.93815600	-4.41153700
H	-3.42221300	2.29929300	-4.75321600
H	-4.62139200	1.64284000	-1.99913700
H	-4.02689200	3.22041100	-2.52866800
H	-2.39144000	2.03432600	-1.06945400
H	-1.71457100	2.35448700	-2.67980500
H	1.49141500	-2.51461400	-1.67292100
H	0.60601000	-2.92851800	-0.21437700
H	1.42279300	-4.97103500	-1.35214300
H	0.60698100	-4.51349300	-2.85360200
H	-0.75746900	-5.20795600	-0.18758600
H	-0.76652100	-6.19983100	-1.65218400
H	-2.90578400	-4.87681800	-1.39116900

H	-2.04318500	-4.45384300	-2.87583900
H	-2.02296800	-2.86956800	-0.23581000
H	-2.86228000	-2.41994200	-1.71212200

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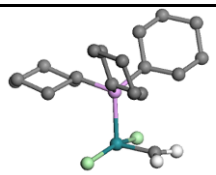
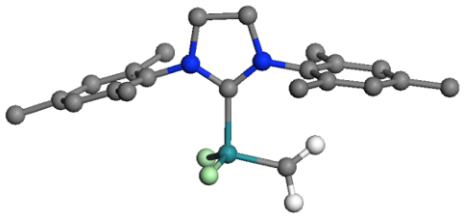


Energy: -6451.301794

C	-0.09605200	0.94799400	1.20287900
Cl	1.93193700	-1.39966200	0.84100700
Ru	-0.38144500	-0.81680600	0.77784700
Cl	-2.70953400	-0.76383900	1.29978700
H	-0.92528000	1.61877800	1.47948600
H	0.92106700	1.36243300	1.29307500
P	-0.57019200	-0.54645800	-1.51907600
C	1.01352800	0.00761800	-2.35876900
C	-2.08104000	0.43087200	-2.05081400
C	-0.87365200	-2.28260000	-2.18363000
C	1.08086700	-0.18427400	-3.88916400
C	2.50928100	0.07713400	-4.40078600
C	3.01451100	1.46873100	-4.00240300
C	2.89921100	1.68881400	-2.48908400
C	1.46958400	1.43170000	-1.98489200
C	-2.49737500	0.30356800	-3.53228300
C	-3.87935000	0.94456300	-3.75710700
C	-3.91117700	2.41009700	-3.30626800
C	-3.44445800	2.55306500	-1.85286400
C	-2.06253400	1.91550200	-1.63413600
C	0.30622300	-3.24190200	-1.92258000
C	0.05613100	-4.61375200	-2.56951500
C	-1.26464200	-5.23382100	-2.09812800
C	-2.43832300	-4.27607100	-2.33264400
C	-2.19625400	-2.90274600	-1.68447800
H	1.73676300	-0.68108000	-1.88863800
H	-2.85350800	-0.05332000	-1.42876200
H	-0.96069300	-2.14716900	-3.27603900
H	0.77303100	-1.19835100	-4.18161200
H	0.38882700	0.51515000	-4.38422300
H	2.53423700	-0.04246900	-5.49635200
H	3.18648100	-0.68994600	-3.98599600
H	2.41978400	2.23670200	-4.52874100
H	4.05797500	1.60198100	-4.33091400
H	3.20084400	2.71570900	-2.22622600
H	3.58974400	1.01200900	-1.95754100
H	0.78993600	2.17436500	-2.43132800
H	1.43407100	1.56879400	-0.89673100
H	-1.75748600	0.80774900	-4.17334500
H	-2.53110800	-0.74782000	-3.85173000
H	-4.63646100	0.37138400	-3.19407300
H	-4.15205800	0.86392100	-4.82218600
H	-4.92644500	2.82227300	-3.42418600
H	-3.25291500	3.00883600	-3.96122600
H	-4.17058700	2.06954200	-1.17746000
H	-3.40823300	3.61615800	-1.56431800
H	-1.77865800	2.01037200	-0.57837500
H	-1.31434500	2.46475800	-2.22667100
H	1.24826200	-2.82279500	-2.30097100
H	0.45061100	-3.36835000	-0.83769300
H	0.90027000	-5.28199500	-2.33647400
H	0.03724500	-4.50354000	-3.66910200
H	-1.19399700	-5.46773400	-1.02137400
H	-1.44253700	-6.18980300	-2.61648200
H	-3.37042400	-4.70485500	-1.93158400
H	-2.59418400	-4.14674800	-3.41958300

H	-2.16573500	-3.01396600	-0.58916500
H	-3.04807000	-2.24160200	-1.89289000

2mB i



Energy: -6329.582571

N	-0.94539200	0.46502200	-0.52409000
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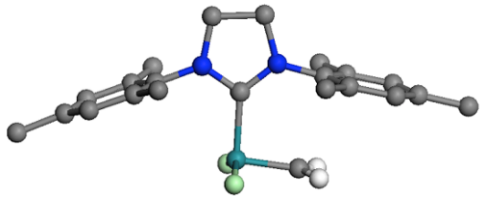
N	1.13518600	-0.25309200	-0.51384500
C	0.82723200	-0.12671500	-1.95651900
C	-0.62472800	0.35993800	-1.96264400
C	-2.29538600	0.80329400	-0.14335300
C	2.43189800	-0.76538100	-0.16902500
C	-3.25949500	-0.22228600	-0.03404600
C	-4.57112700	0.13674800	0.29735400
C	-4.95222600	1.46888500	0.49631000
C	-3.98560400	2.46315900	0.30903000
C	-2.65800200	2.16231700	-0.02463500
C	3.51757700	0.12496400	-0.06095400
C	4.78810000	-0.41503600	0.18479200
C	5.00039600	-1.79177200	0.32304600
C	3.89440000	-2.64576900	0.20898400
C	2.60425500	-2.16017400	-0.03811800
C	-2.93285800	-1.66532000	-0.32042800
H	-5.31781800	-0.65447700	0.40447800
C	-6.35606800	1.81978000	0.92037800
H	-4.26822200	3.51280800	0.42532700
C	-1.68181400	3.27931600	-0.28944500
C	3.32912400	1.61518300	-0.17713400
H	5.63727700	0.26768800	0.27453300
C	6.37577200	-2.34033800	0.61349800
H	4.03723600	-3.72450000	0.31837200
C	1.43275800	-3.10705500	-0.11592800
H	-3.70879000	-2.32613700	0.08756300
H	-1.97875500	-1.96821800	0.12377100
H	-2.88506300	-1.84981300	-1.40759900
H	-6.43746300	1.82396100	2.02003100
H	-7.08830000	1.09237300	0.54146000
H	-6.64988800	2.81866400	0.56695400
H	-2.13591000	4.25057100	-0.05028800
H	-1.38757700	3.30933100	-1.35199700
H	-0.76837900	3.17598100	0.31063500
H	4.27738100	2.14163200	-0.00343400
H	2.59425000	1.98289500	0.55387700
H	2.96985600	1.90785900	-1.17664800
H	6.49964400	-2.54403900	1.68996000
H	7.16209400	-1.63160900	0.31928700
H	6.55230900	-3.28610800	0.08057700
H	1.76513400	-4.14795100	-0.00504200
H	0.90053500	-3.02790100	-1.07599100
H	0.70005700	-2.89775400	0.67778100
H	0.95743400	-1.09694800	-2.45756600
H	-1.31027100	-0.34754600	-2.45072700
H	1.51767600	0.58964600	-2.42457400
H	-0.74149400	1.33803000	-2.45001900
Ru	-0.03469300	0.26260200	2.28023000
Cl	-1.65398200	-1.33702700	2.83364100
Cl	0.49233000	2.54966000	2.39869900
C	1.50841400	-0.54394400	2.85594400
H	1.66783100	-0.49596500	3.95131700

H	2.27155300	-1.07714100	2.28098100

2mB a



Energy: -6329.574876

C	-0.30759400	1.70437300	-1.12510700
Ru	-0.08438000	-0.11575200	-0.92162900
Cl	2.27826100	0.10821000	-0.65826100
Cl	-2.36556800	-0.43188900	-0.29234300
H	0.55103500	2.38295700	-1.23491300
H	-1.29479000	2.17875800	-1.01821000
N	-0.08524800	-1.79714900	-3.32479300
C	-0.19304200	-0.52226800	-2.86374800
N	-0.39010600	0.30358600	-3.92739300
C	-0.42626000	-0.42576800	-5.21468000
C	-0.20153100	-1.88815300	-4.79496800
C	0.14218200	-2.96983300	-2.51588500
C	-0.55711400	1.72763300	-3.90612100
C	-0.96857700	-3.72261500	-2.07167000
C	-0.71892400	-4.87049800	-1.30969400
C	0.57807600	-5.29526700	-1.00211900
C	1.65234200	-4.55955600	-1.51407200
C	1.46589500	-3.40367200	-2.28256000
C	0.57671300	2.55496100	-4.07573600
C	0.37711400	3.93800100	-4.14921400
C	-0.89864500	4.51126600	-4.06498200
C	-1.99984500	3.66013800	-3.91447800
C	-1.86119200	2.26887600	-3.83781900
C	2.65703000	-2.67475500	-2.84710600
C	-2.38431800	-3.33224500	-2.40674800
C	0.80863700	-6.50246400	-0.12727500
C	-3.06751600	1.38595100	-3.65775600
C	1.96593800	1.97634800	-4.14297000
C	-1.07590300	6.00870000	-4.10923700
H	0.35871700	-0.05238300	-5.88778100
H	0.71442200	-2.31810400	-5.22419000
H	-1.57088300	-5.45085800	-0.94601800
H	2.67334700	-4.89124800	-1.31037700
H	1.24798500	4.58713000	-4.27298800
H	-3.00338300	4.08979200	-3.85334600
H	3.58758400	-3.18910800	-2.57240900
H	2.71438900	-1.64690000	-2.46117700
H	2.61863500	-2.62477500	-3.94700800
H	-3.09076700	-4.08035800	-2.02236100
H	-2.53894700	-3.25911100	-3.49476600
H	-2.64531600	-2.36111000	-1.96150100
H	-0.00216300	-7.23757000	-0.23024600
H	0.84987200	-6.20639300	0.93377000
H	1.75829400	-7.00223200	-0.36535000
H	-3.00576400	0.81293600	-2.71898700
H	-3.16884900	0.65658300	-4.47637300
H	-3.98747800	1.98550500	-3.63164700
H	2.71093600	2.77096300	-4.28382600
H	2.07560900	1.26522800	-4.97635400
H	2.21605000	1.43127200	-3.21910500
H	-0.31802200	6.48612800	-4.74584300
H	-0.97602000	6.44279300	-3.10044300
H	-2.06893300	6.28872000	-4.48796400
H	-1.39594800	-0.27420200	-5.70982700
H	-1.04449400	-2.53786800	-5.06900600

1mBi (Ru-organophosphine at 20Å taken as the reference state for dissociation energy)

Energy: -7498.5947317

C	0.06357000	2.18779000	0.83946800
Ru	0.11188200	0.35202000	0.81684700
Cl	-1.98067000	-0.34485700	1.59948100
Cl	2.38018100	-0.22422300	0.82339000
P	3.27000200	-3.04338400	20.27297200
C	1.89118200	-2.42913500	21.42587300
C	3.30580100	-4.89086200	20.68905600
C	4.96207100	-2.46983500	20.90431400
C	5.25098300	-1.00512700	20.51228200
C	6.73720300	-0.66167300	20.71469300
C	7.19478300	-0.94785600	22.15118400
C	6.87831100	-2.39082900	22.56669000
C	5.38874300	-2.72409000	22.36089300
C	1.64680800	-0.91586100	21.27554300
C	0.30639300	-0.50592400	21.91954300
C	0.23424000	-0.93895700	23.38791200
C	0.52230100	-2.43320100	23.56143800
C	1.86609900	-2.82708300	22.91125100
C	1.95569000	-5.54180600	20.32296600
C	1.95154600	-7.05994300	20.57184000
C	3.09789400	-7.75559300	19.83143500
C	4.44682700	-7.12404000	20.18866900
C	4.44789100	-5.60538500	19.93817100
H	1.02302400	-2.92044200	20.94638500
H	3.47146200	-5.02805900	21.77252300
H	5.62304400	-3.08334800	20.26299500
H	4.95976200	-0.82831700	19.46460700
H	4.63851400	-0.32756800	21.12977400
H	6.91995300	0.39432700	20.45677600
H	7.34057300	-1.26897500	20.01607100
H	6.69059800	-0.24855500	22.84291300
H	8.27587100	-0.75056600	22.25377500
H	7.16097700	-2.56004100	23.61873900
H	7.48730300	-3.08317500	21.95781800
H	4.78701700	-2.09340200	23.03455400
H	5.19787700	-3.76865100	22.65053000
H	2.46153400	-0.35685800	21.76548100
H	1.65796800	-0.62638000	20.21275400
H	-0.50781400	-1.00109900	21.36147300
H	0.16033000	0.58120000	21.82570800
H	-0.76340100	-0.69790400	23.80162200
H	0.94054700	-0.34372600	23.99435600
H	-0.28017900	-3.00854800	23.06673500
H	0.52293800	-2.71134400	24.62640400
H	2.02725700	-3.90847200	23.03812700
H	2.68391700	-2.32239600	23.44916800
H	1.13390400	-5.08379500	20.89306400
H	1.74190900	-5.34594400	19.25675100
H	0.97997300	-7.48091500	20.26697700
H	2.05736000	-7.24283600	21.65628500
H	2.93278400	-7.68587800	18.74126500
H	3.10659000	-8.83395000	20.06775900
H	5.26104300	-7.59494800	19.61474300
H	4.65845300	-7.30735800	21.25740500
H	4.34435000	-5.41346700	18.85489700
H	5.42545200	-5.19810700	20.23606100
P	-0.28225700	-0.03392700	-1.41206300
C	1.11432300	0.59513800	-2.51644000
C	-0.31853800	-1.88461600	-1.79457700
C	-1.98723400	0.54006300	-1.98038000
C	-2.32514400	2.00642300	-1.64326300
C	-3.79985500	2.31907300	-1.94953200
C	-4.16764200	1.99439200	-3.40171800
C	-3.82610300	0.53785000	-3.73471400

C	-2.34589600	0.23010600	-3.44979000
C	1.31742500	2.12255500	-2.46798300
C	2.61610800	2.53394800	-3.18142500
C	2.66048000	2.02945000	-4.62772800
C	2.43809400	0.51412900	-4.68111900
C	1.12923700	0.10590700	-3.98221000
C	1.02548100	-2.58907800	-1.51501800
C	0.98436200	-4.06147400	-1.95686600
C	-0.16679900	-4.82151600	-1.28867900
C	-1.50363700	-4.11934900	-1.54869000
C	-1.47154300	-2.64583700	-1.10771200
H	1.98277200	0.14937600	-2.00109600
H	-0.49655800	-1.92795900	-2.88282700
H	-2.63166000	-0.07666800	-1.33094900
H	-2.12983400	2.19580500	-0.58036900
H	-1.68373700	2.68516500	-2.22901000
H	-4.00302600	3.37907900	-1.72649300
H	-4.43767100	1.72738100	-1.27018500
H	-3.60806800	2.66330200	-4.08039600
H	-5.23789400	2.18823800	-3.58018600
H	-4.04890300	0.31814000	-4.79172800
H	-4.46125700	-0.13435200	-3.13137900
H	-1.72692500	0.85040400	-4.11592500
H	-2.13411000	-0.81877100	-3.70114800
H	0.46520400	2.62888200	-2.95069100
H	1.35854300	2.46236700	-1.42588300
H	3.47434500	2.12143900	-2.62316200
H	2.71952100	3.63091000	-3.15053800
H	3.62247600	2.29198600	-5.09714400
H	1.87411100	2.53448700	-5.21715400
H	3.28559000	0.00211100	-4.19262300
H	2.41829500	0.16238700	-5.72591700
H	1.01368700	-0.98507300	-4.04233800
H	0.28450600	0.54743400	-4.53174700
H	1.85581400	-2.07882300	-2.02243900
H	1.25138500	-2.53599800	-0.43966200
H	1.94981600	-4.53789300	-1.72092300
H	0.86870900	-4.11441000	-3.05487300
H	0.01235700	-4.87290500	-0.20053700
H	-0.20159600	-5.86173800	-1.65207400
H	-2.32221200	-4.63612300	-1.02185000
H	-1.74209000	-4.17471500	-2.62662700
H	-1.35209300	-2.58974900	-0.01571700
H	-2.44141600	-2.18096400	-1.33228700
H	0.23792700	2.63351300	1.83820200
H	-0.11479200	2.90183000	0.02675900

1mBa (Ru-organophosphine at 20Å taken as the reference state for dissociation energy)

Energy: -7498.576060

C	-0.09634000	0.94674900	1.20042500
Cl	1.93170300	-1.39630000	0.84178300
Ru	-0.38211000	-0.81740000	0.77572500
Cl	-2.70913000	-0.76105000	1.29932700
H	-0.92519000	1.61773300	1.47652400
H	0.92052500	1.36156000	1.28765700
P	-0.56942000	-0.54631000	-1.52110000
C	1.01329000	0.00731200	-2.35953000
C	-2.07870000	0.43060800	-2.05230000
C	-0.87292000	-2.28173000	-2.18654000
C	1.07816300	-0.17949000	-3.89035000
C	2.50552400	0.08097600	-4.40308000
C	3.01393000	1.46997900	-4.00056000
C	2.90026100	1.68566700	-2.48714000
C	1.47118000	1.42943200	-1.98261000
C	-2.49416000	0.30640800	-3.53397000
C	-3.87687000	0.94476700	-3.75692000
C	-3.91138000	2.40875900	-3.30244000
C	-3.44370000	2.54972100	-1.84974000
C	-2.06124000	1.91400100	-1.63328000
C	0.30523900	-3.24159000	-1.92042000
C	0.05613700	-4.61542000	-2.56199000
C	-1.26494000	-5.23314000	-2.08977000
C	-2.43667000	-4.27612000	-2.33265000
C	-2.19682000	-2.90066000	-1.68942000
H	1.73623000	-0.68357000	-1.89330000
H	-2.85156000	-0.05486000	-1.43248000
H	-0.95743000	-2.14778000	-3.27881000
H	0.76771600	-1.19153000	-4.18567000
H	0.38735200	0.52332300	-4.38133000
H	2.52852000	-0.03440000	-5.49882000
H	3.18200500	-0.68864000	-3.99286000
H	2.42058500	2.24067600	-4.52379000
H	4.05712200	1.60187100	-4.32913000
H	3.20460600	2.71058800	-2.22117000
H	3.58915100	1.00551900	-1.95844000
H	0.79142200	2.17364400	-2.42538000
H	1.43754800	1.56313300	-0.89429000
H	-1.75585000	0.81463100	-4.17297000
H	-2.52499000	-0.74385000	-3.85620000
H	-4.63257000	0.36892200	-3.19554000
H	-4.14961000	0.86674400	-4.82182000
H	-4.92742000	2.81867300	-3.41806000
H	-3.25535000	3.00982500	-3.95689000
H	-4.16784000	2.06295700	-1.17504000
H	-3.40979000	3.61176200	-1.55841000
H	-1.77740000	2.00677100	-0.57766000
H	-1.31368000	2.46453200	-2.22479000
H	1.24834900	-2.82498000	-2.29812000
H	0.44705500	-3.36437000	-0.83532000
H	0.89971000	-5.28247000	-2.32478000
H	0.03793900	-4.50974000	-3.66161000
H	-1.19656000	-5.46164000	-1.01214000
H	-1.44208000	-6.19120000	-2.60383000
H	-3.37024000	-4.70248000	-1.93314000
H	-2.58767000	-4.15158000	-3.42030000
H	-2.16945000	-3.00785000	-0.59407000
H	-3.04815000	-2.24110000	-1.90334000
P	1.03701500	-7.01801000	19.73016000
C	-0.32491000	-6.40138000	20.90094000
C	0.80281500	-8.89543000	19.82464000
C	2.73024700	-6.79002000	20.55468000
C	3.22552600	-5.33498000	20.41693000
C	4.70904000	-5.20891000	20.79536000

C	4.98307000	-5.75337000	22.20308000
C	4.47798300	-7.19362000	22.35445000
C	2.99156600	-7.31459000	21.97708000
C	-0.31132000	-4.86332000	21.00698000
C	-1.58526000	-4.33264000	21.68075000
C	-1.80325000	-4.97397000	23.05676000
C	-1.80099000	-6.50459000	22.96417000
C	-0.52186000	-7.03145000	22.29164000
C	-0.59040000	-9.27381000	19.27937000
C	-0.80509000	-10.79410000	19.22347000
C	0.29218300	-11.49250000	18.41407000
C	1.68036700	-11.13520000	18.95497000
C	1.89779400	-9.61519000	19.00967000
H	-1.22417000	-6.65347000	20.30723000
H	0.87156200	-9.23896000	20.87112000
H	3.36647200	-7.38427000	19.87201000
H	3.06022800	-4.97959000	19.38784000
H	2.63327900	-4.67719000	21.07263000
H	5.02839400	-4.15644000	20.72486000
H	5.31730400	-5.76879000	20.06326000
H	4.47457800	-5.11253000	22.94489000
H	6.05935900	-5.69960000	22.43257000
H	4.63337400	-7.54757000	23.38672000
H	5.07292600	-7.85902000	21.70439000
H	2.39616200	-6.73393000	22.69826000
H	2.66515800	-8.36117000	22.07083000
H	0.56193300	-4.54526000	21.59962000
H	-0.19118000	-4.41770000	20.00649000
H	-2.45356000	-4.55130000	21.03422000
H	-1.53321000	-3.23557000	21.77297000
H	-2.74658000	-4.61777000	23.50169000
H	-0.99672000	-4.65113000	23.73891000
H	-2.67954000	-6.83390000	22.38082000
H	-1.90868000	-6.94974000	23.96736000
H	-0.56544000	-8.12860000	22.22074000
H	0.34056800	-6.79425000	22.93257000
H	-1.38176000	-8.81939000	19.89441000
H	-0.70253000	-8.85019000	18.26588000
H	-1.79641000	-11.01450000	18.79440000
H	-0.81246000	-11.19880000	20.25090000
H	0.21977600	-11.18010000	17.35763000
H	0.14513700	-12.58450000	18.42982000
H	2.46659000	-11.60130000	18.33808000
H	1.79342700	-11.55350000	19.97053000
H	1.90698100	-9.20650000	17.98374000
H	2.89042400	-9.40921000	19.43699000

2mBi (Ru-organophosphine at 20Å taken as the reference state for dissociation energy)

Energy: -7376.8571771

C	-0.42966700	1.74313800	-0.87509200
Ru	0.12728500	-0.00425100	-0.88576700
Cl	-0.25381800	-0.64743100	1.33622000
Cl	-0.17636200	-0.64465100	-3.12565500
P	-19.34814700	-3.60264400	1.92978200
C	-20.43970600	-3.39896900	0.39464400
C	-19.58636700	-5.43351200	2.34924000
C	-20.16061200	-2.76001200	3.42171200
C	-20.06899600	-1.22244500	3.32378100
C	-20.42438200	-0.55437000	4.66188100
C	-21.80991000	-0.98876600	5.15841200
C	-21.91807900	-2.51750100	5.23815400
C	-21.56457100	-3.18001300	3.89459900
C	-20.31128500	-1.98135500	-0.20279200
C	-20.90725600	-1.91692400	-1.61816200
C	-22.36689500	-2.39144000	-1.63865500
C	-22.51141800	-3.78823800	-1.01868900
C	-21.91424000	-3.84379400	0.39909200
C	-19.14657400	-6.32995600	1.17195500
C	-19.21862300	-7.82624300	1.51902200
C	-18.40243700	-8.15992900	2.77257900
C	-18.83702400	-7.28514500	3.95357300
C	-18.76820600	-5.78824200	3.61008400
H	-19.90742800	-4.06493300	-0.31156000
H	-20.65042800	-5.64210600	2.55838300
H	-19.45239300	-3.05060500	4.22132400
H	-19.05888500	-0.92210900	3.00201200
H	-20.76816400	-0.86084100	2.55222800
H	-20.37985500	0.54275000	4.55820800
H	-19.66441900	-0.83006000	5.41529000
H	-22.57911300	-0.60812500	4.46210900
H	-22.02483500	-0.53621900	6.14071000
H	-22.93366200	-2.81514600	5.54913600
H	-21.22877400	-2.89037600	6.01730100
H	-22.31200400	-2.87923200	3.14418300
H	-21.63697500	-4.27403800	3.99070300
H	-20.84225700	-1.25915500	0.43844800
H	-19.25429500	-1.67093500	-0.21745600
H	-20.30439100	-2.55295700	-2.29116100
H	-20.83548500	-0.88861800	-2.01076400
H	-22.75640600	-2.38816900	-2.67035800
H	-22.98716600	-1.67783500	-1.06664600
H	-21.99405800	-4.52659200	-1.65764000
H	-23.57266200	-4.08802800	-0.99307000
H	-22.01595700	-4.86107700	0.80749000
H	-22.49985600	-3.18090900	1.05532300
H	-19.77044500	-6.13879100	0.28625300
H	-18.11103600	-6.06945100	0.88869100
H	-18.86675300	-8.42287800	0.66073300
H	-20.27362000	-8.10896800	1.68603400
H	-17.33055200	-7.98850800	2.56601200
H	-18.50682700	-9.22797400	3.02599900
H	-18.21002200	-7.49058000	4.83729800
H	-19.87245400	-7.54550500	4.23793200
H	-17.71488300	-5.49992200	3.44393400
H	-19.11958800	-5.20532200	4.47461100
H	0.16511300	2.65973500	-0.81441300
H	-1.52902900	1.87543300	-0.90566000
N	2.94809300	-0.90514100	-0.83676700
C	2.11875800	0.17507300	-0.96148400
N	2.90219000	1.26121000	-1.22203900
C	4.34638800	0.93867000	-1.27225300
C	4.37275300	-0.57599900	-1.04938600
C	2.60124100	-2.25255200	-0.45527600

C	2.53873700	2.64331800	-1.36622900
C	2.40328000	-3.23153300	-1.45260900
C	2.11187300	-4.53952100	-1.04286900
C	2.04692900	-4.90158000	0.30728700
C	2.31392100	-3.91753800	1.26604400
C	2.60964700	-2.59534800	0.91454200
C	2.50993400	3.46291500	-0.21863500
C	2.24548000	4.82762500	-0.38848400
C	2.02143900	5.38949300	-1.65273800
C	2.06296100	4.54397800	-2.76807700
C	2.32112700	3.17095300	-2.65420100
C	2.98154200	-1.60224700	1.98511500
C	2.54955200	-2.92484500	-2.92080200
C	1.68306000	-6.30660600	0.71811200
C	2.33753800	2.29347400	-3.87966800
C	2.71291000	2.89051500	1.16189200
C	1.71408300	6.85906500	-1.80483200
H	4.88369800	1.49437800	-0.48953900
H	4.96295100	-0.86470800	-0.16856700
H	1.94130400	-5.29994600	-1.80962400
H	2.29759200	-4.18569400	2.32548600
H	2.21450600	5.47084700	0.49510300
H	1.89001200	4.96345700	-3.76270800
H	2.68992600	-1.97527300	2.97553900
H	2.48420900	-0.63745600	1.83810100
H	4.07154400	-1.43262100	2.00546200
H	2.26351200	-3.79593900	-3.52549200
H	3.59416500	-2.68076300	-3.17557700
H	1.92012000	-2.08004800	-3.22835800
H	2.01789400	-7.04518800	-0.02435500
H	0.58984100	-6.41157200	0.81663700
H	2.12588700	-6.57143500	1.68895700
H	1.56809000	1.50940800	-3.81925600
H	3.30526500	1.78480800	-4.01028000
H	2.15203500	2.88792800	-4.78453300
H	2.68304100	3.68481100	1.91989700
H	3.68078000	2.37613600	1.26022900
H	1.93192300	2.15570300	1.40882600
H	2.22508400	7.45984400	-1.03921700
H	0.63229700	7.04589600	-1.70072000
H	2.01803600	7.23269100	-2.79280200
H	4.76255900	1.23576000	-2.24512800
H	4.76382700	-1.12500800	-1.91809300

2mBa (Ru-organophosphine at 20Å taken as the reference state for dissociation energy)

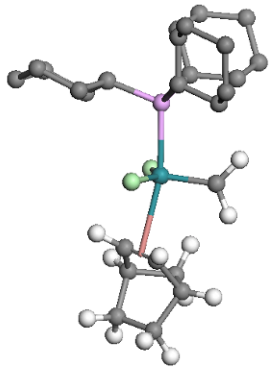
Energy: -7376.8493509

C	-0.28942500	1.69654300	-1.13062100
Ru	-0.05422800	-0.12254400	-0.93033800
Cl	2.31024200	0.12405500	-0.66495700
Cl	-2.32493200	-0.43847600	-0.26781600
P	1.17143400	2.40466700	18.88314600
C	-0.37186000	2.98293200	19.81770500
C	1.48218200	0.71060300	19.67111800
C	2.67537700	3.39443900	19.47936600
C	2.60152000	4.86788100	19.02634400
C	3.95615400	5.57338700	19.20435600
C	4.46737900	5.46611900	20.64759700
C	4.50943900	4.00712000	21.12180600
C	3.14607700	3.31519100	20.94471600
C	-1.01926600	4.20958100	19.13877300
C	-2.42675900	4.47573200	19.69837700
C	-2.41276200	4.63506900	21.22472000
C	-1.74462400	3.43356100	21.90658800
C	-0.33510800	3.17870100	21.34372100
C	0.32201100	-0.25963700	19.36056800
C	0.58020500	-1.67101700	19.91326700
C	1.90355100	-2.24779200	19.39672700
C	3.06737500	-1.29730800	19.69808700
C	2.80759400	0.11495300	19.14825300
H	-1.05849700	2.13904600	19.61797400
H	1.55918600	0.81199100	20.76830400
H	3.47261600	2.93335500	18.86490000
H	2.27741900	4.92438700	17.97462200
H	1.84024900	5.39931900	19.62143000
H	3.87322700	6.63215700	18.90630000
H	4.69261800	5.11426000	18.52046000
H	3.80042100	6.04462600	21.31223900
H	5.46618400	5.92554200	20.73374000
H	4.82243400	3.95886900	22.17849600
H	5.27379600	3.45681100	20.54389000
H	2.41026800	3.80600900	21.59923500
H	3.21486700	2.26929800	21.28069300
H	-0.39324500	5.10198700	19.30494800
H	-1.06461700	4.05699600	18.04877200
H	-3.08621100	3.63159200	19.42689600
H	-2.85875000	5.37275700	19.22394800
H	-3.43864900	4.77014500	21.60581800
H	-1.85697000	5.55384500	21.48649000
H	-2.36457100	2.53241000	21.74966400
H	-1.69199300	3.59129100	22.99699700
H	0.11669400	2.30699000	21.84147800
H	0.29992700	4.04619700	21.58420600
H	-0.62410800	0.11903600	19.77453200
H	0.18608300	-0.31514700	18.26572000
H	-0.25928900	-2.33406900	19.64539800
H	0.60752900	-1.62883700	21.01707400
H	1.83135000	-2.40051200	18.30489600
H	2.09045800	-3.23902800	19.84198800
H	4.00675400	-1.69306300	19.27723700
H	3.21394600	-1.23804600	20.79164500
H	2.76991500	0.07628800	18.04473700
H	3.65591200	0.76418300	19.40986500
H	0.56556300	2.37952000	-1.24529100
H	-1.27642900	2.16654300	-1.00614100
N	-0.05272400	-1.79713700	-3.33835200
C	-0.16664600	-0.52476200	-2.87288700
N	-0.36609800	0.30408000	-3.93288400
C	-0.41207900	-0.42204500	-5.22168000
C	-0.15985400	-1.88216300	-4.80974700
C	0.15361700	-2.97438200	-2.53021200

C	-0.55006300	1.72635600	-3.90741600
C	-0.96944700	-3.71216100	-2.09223900
C	-0.74034000	-4.85809900	-1.32017800
C	0.54936900	-5.29416300	-0.99581400
C	1.63674000	-4.57508500	-1.50491500
C	1.47076100	-3.42284000	-2.28454100
C	0.57378900	2.56767400	-4.08017900
C	0.35726400	3.94822900	-4.15291600
C	-0.92545000	4.50665400	-4.06200800
C	-2.01553400	3.64209200	-3.90313800
C	-1.85985600	2.25202400	-3.82780600
C	2.67673400	-2.71080400	-2.83755400
C	-2.37773800	-3.30153400	-2.43247100
C	0.75941400	-6.49358100	-0.10630600
C	-3.05407700	1.35495900	-3.63728800
C	1.96917800	2.00484700	-4.14895900
C	-1.11877500	6.00170200	-4.10804300
H	0.35769400	-0.03637100	-5.90514200
H	0.76871100	-2.28810200	-5.23611100
H	-1.60254100	-5.42618400	-0.96127300
H	2.65245500	-4.91751600	-1.29093000
H	1.22000300	4.60789600	-4.27816900
H	-3.02358700	4.05975800	-3.83483900
H	3.58378500	-3.30816700	-2.67204100
H	2.81840200	-1.73609400	-2.34656500
H	2.58911400	-2.53275400	-3.92009200
H	-3.09191500	-4.06715200	-2.10038200
H	-2.51684900	-3.16432300	-3.51614600
H	-2.64105600	-2.35571000	-1.93538700
H	-0.05952000	-7.22024700	-0.20588000
H	0.79739500	-6.18604100	0.95176000
H	1.70428300	-7.00820300	-0.33206400
H	-2.96333000	0.75875900	-2.71584100
H	-3.17264400	0.64762700	-4.47301800
H	-3.97760000	1.94568000	-3.56983400
H	2.70916700	2.81150700	-4.23761300
H	2.10049700	1.33754000	-5.01538200
H	2.20845100	1.42040300	-3.24697200
H	-0.40284000	6.47763900	-4.79355600
H	-0.96271100	6.44739700	-3.11174100
H	-2.13391500	6.27065500	-4.43176800
H	-1.39158200	-0.28245800	-5.70143500
H	-0.98490500	-2.55028000	-5.09360600

Stage C

1mCa

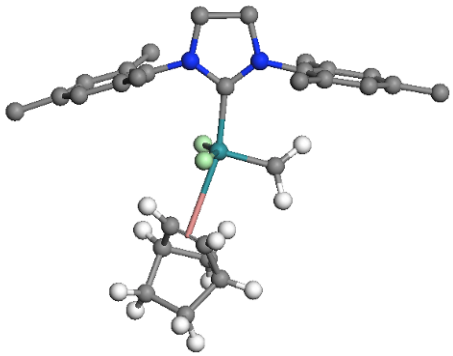


Energy: -6724.091625

C	-0.16201100	1.90950000	0.41673400
Cl	2.07596800	-0.57412500	0.39566900
Ru	-0.21024600	0.06812600	0.53947200
Cl	-2.48782700	-0.51948100	0.91750200
H	-0.01449100	2.49218100	1.33989900
H	-0.25304000	2.50865000	-0.49779300
P	-0.50904800	-0.34984700	-1.77660100
C	0.95704100	0.18073000	-2.84907300
C	-2.13557500	0.28536900	-2.48600200
C	-0.62720500	-2.21192800	-2.11615000
C	1.15979300	-0.53457300	-4.20349400
C	2.49759300	-0.12390900	-4.84481000
C	2.60792100	1.39423800	-5.02458800
C	2.37411200	2.11773300	-3.69439900
C	1.03940400	1.70860400	-3.05027700
C	-2.37741200	-0.00002300	-3.98238000
C	-3.82628700	0.33677200	-4.37854700
C	-4.17448400	1.79249700	-4.04594300
C	-3.91046800	2.09393300	-2.56643800
C	-2.46807600	1.75433100	-2.15416900
C	0.60042500	-2.98563800	-1.59300700
C	0.55787200	-4.46344800	-2.01285100
C	-0.73495400	-5.14316600	-1.54994600
C	-1.96452800	-4.37159900	-2.04098900
C	-1.92355600	-2.88983200	-1.62625500
H	1.79803500	-0.09902400	-2.19192700
H	-2.85253900	-0.31444300	-1.90148200
H	-0.62313300	-2.28367700	-3.21688500
H	1.15096300	-1.62569600	-4.08131400
H	0.33863200	-0.28367200	-4.89328900
H	2.61163100	-0.63700400	-5.81407500
H	3.32491500	-0.47559800	-4.20378900
H	1.85734800	1.73093800	-5.76237800
H	3.59480900	1.66045100	-5.43760600
H	2.39245900	3.21026700	-3.84092600
H	3.19576900	1.87911100	-2.99726900
H	0.21387400	2.04271400	-3.69979500
H	0.93078300	2.22954500	-2.09104000
H	-1.69472900	0.61384500	-4.59179100
H	-2.16499000	-1.05079400	-4.22749900
H	-4.51483200	-0.33782200	-3.83950000
H	-3.97012300	0.14096400	-5.45425000
H	-5.22638500	2.00321100	-4.29897100
H	-3.55980700	2.46308600	-4.67338700
H	-4.60309600	1.50266000	-1.94257600

H	-4.11696400	3.15413700	-2.34596700
H	-2.35416200	1.92112700	-1.07507500
H	-1.77351700	2.43354400	-2.67455100
H	1.53792700	-2.52740700	-1.93547700
H	0.62783700	-2.92375800	-0.49470300
H	1.43634300	-4.98263300	-1.59553800
H	0.64055200	-4.53911300	-3.11236400
H	-0.74843900	-5.18441600	-0.44629500
H	-0.76946200	-6.18695100	-1.90360300
H	-2.88719300	-4.82906400	-1.64761000
H	-2.02472400	-4.44367900	-3.14230400
H	-1.99639900	-2.80728800	-0.53242500
H	-2.81066500	-2.38459400	-2.03211300
C	0.14330600	-0.62879000	3.07120500
C	-0.48829400	0.56689100	3.24474300
H	-0.33935900	-1.56726000	2.79317800
C	1.48289700	-0.54027300	3.77921200
H	-1.54927800	0.75711800	3.09051600
C	0.44143500	1.44694500	4.06039900
C	1.82354700	0.95266800	3.58859700
C	0.39504800	0.81752800	5.50047600
C	1.10667300	-0.55582800	5.30378000
H	2.23935300	-1.26955500	3.47081800
H	0.24726400	2.52690600	4.03708300
H	2.64344800	1.29042400	4.24053700
H	2.05194700	1.19584700	2.54422000
H	-0.63282600	0.72205600	5.87830300
H	0.94879200	1.45954700	6.20271200
H	0.46478100	-1.41054200	5.55953400
H	2.01944200	-0.62843800	5.91445300

2mCi

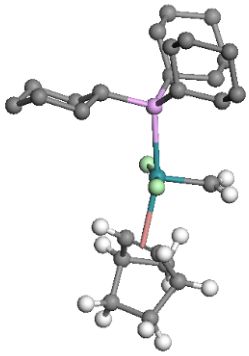


Energy: -6602.351244

N	-0.82800500	0.40700200	-0.92065400
C	0.18608100	0.02434500	-0.08623700
N	1.24620700	-0.30341600	-0.87644900
C	0.94468800	-0.21669200	-2.32600300
C	-0.44239200	0.42637500	-2.34650300
C	-2.16082900	0.82275300	-0.55904200
C	2.54515200	-0.80272300	-0.51843000
C	-3.19590500	-0.13824900	-0.53356000
C	-4.48028100	0.28105200	-0.16777100
C	-4.77276200	1.61669700	0.12783300
C	-3.74696100	2.55781100	-0.01023400
C	-2.44295500	2.19469500	-0.37299100
C	3.60640600	0.10971400	-0.36138000
C	4.88649500	-0.40751300	-0.11935800
C	5.13060000	-1.78314000	-0.03288900
C	4.04817900	-2.65786200	-0.19221900
C	2.74936700	-2.19597600	-0.43920000
C	-2.99250400	-1.56440600	-0.97653800
H	-5.27731900	-0.46589800	-0.11975000
C	-6.15093900	2.02921200	0.58257700
H	-3.96349600	3.61606100	0.16053700
C	-1.43428000	3.27951700	-0.65217100
C	3.38187200	1.59817000	-0.43181800
H	5.71830800	0.29095700	0.00496200
C	6.51553100	-2.31022400	0.25439500
H	4.21513300	-3.73616700	-0.12089200
C	1.60508400	-3.16961000	-0.57413400
H	-3.62928800	-2.24465100	-0.39644500
H	-1.95928500	-1.89898500	-0.84933700
H	-3.27306200	-1.67038800	-2.03955100
H	-6.21028600	2.04382600	1.68358600
H	-6.91955400	1.33007700	0.22365500
H	-6.41203200	3.03753900	0.22966400
H	-1.60184700	4.14738600	-0.00140600
H	-1.53757100	3.62677100	-1.69558000
H	-0.40385000	2.95027000	-0.49089400
H	4.31973300	2.14102400	-0.25155300
H	2.64227600	1.92898700	0.31247000
H	3.00657400	1.90827800	-1.42023400
H	6.65129200	-2.49587400	1.33289000
H	7.28942200	-1.59427500	-0.05625700
H	6.70018000	-3.26017100	-0.26759600
H	1.93740900	-4.19196400	-0.34831200
H	1.19293000	-3.17813700	-1.59605700
H	0.77899600	-2.92108400	0.10844500
H	0.95254400	-1.22424800	-2.76867700
H	-1.16885400	-0.14074900	-2.94411100
H	1.70855800	0.38528400	-2.83586600

H	-0.42430200	1.46366700	-2.71527100
Ru	-0.06727500	0.07990800	1.94112700
Cl	-1.41906100	-1.88770500	1.90038200
Cl	0.39687100	2.42090800	2.04276000
C	1.53560000	-0.65181100	2.46855500
H	1.79625900	-0.59317600	3.53855700
H	2.25138900	-1.18840600	1.83770300
C	-0.32572300	0.74926800	4.82822100
C	-1.55417200	0.60950500	4.26391200
C	-0.24830600	-0.22690000	5.98793800
H	0.37460800	1.56119700	4.63809100
C	-2.29082800	-0.46315300	5.04621900
H	-2.03301600	1.32528300	3.59419600
C	-1.12286300	-1.38367600	5.46051000
C	-1.20877400	0.37997000	7.07478600
C	-2.61639000	0.21596700	6.42452900
H	0.75504600	-0.47663200	6.35742800
H	-3.14356300	-0.93284500	4.54375700
H	-1.40278100	-2.10535300	6.24379500
H	-0.68497500	-1.90925800	4.60324400
H	-0.96052000	1.42518500	7.30716600
H	-1.12563800	-0.19733400	8.00889800
H	-3.14194100	1.17297600	6.29633900
H	-3.26290000	-0.44100300	7.02662500

1mCa

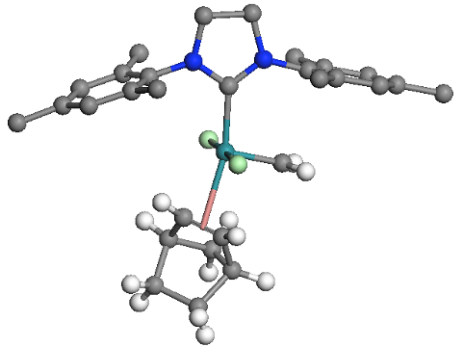


Energy: -6724.088320

C	0.16398200	2.27108000	-0.06732400
Cl	2.17805900	-0.11141000	-0.08861000
Ru	-0.18363200	0.47973400	0.15714100
Cl	-2.61109700	0.70702700	0.38885400
H	-0.61975000	3.02830400	0.10036200
H	1.17130700	2.64354800	-0.31344200
P	-0.51475100	-0.18576900	-2.16467900
C	1.00747200	0.00007300	-3.25080700
C	-2.03852400	0.57272800	-2.95828200
C	-0.86531500	-2.03847000	-2.18691300
C	1.03871500	-0.78948900	-4.57583200
C	2.43880700	-0.71076100	-5.21198200
C	2.88804800	0.73855500	-5.43043800
C	2.81140700	1.54494400	-4.12841600
C	1.41122500	1.46657600	-3.49829000
C	-2.44725900	0.02231500	-4.34030700
C	-3.83662800	0.55243700	-4.73746700
C	-3.88325000	2.08509200	-4.72769800
C	-3.42787200	2.64479600	-3.37413600
C	-2.04114000	2.11346200	-2.97773100
C	0.30888900	-2.86890800	-1.62678200
C	0.03212200	-4.37505200	-1.75114200
C	-1.28161300	-4.77047700	-1.06815700
C	-2.45008000	-3.93424600	-1.60187700
C	-2.18139600	-2.42540900	-1.48121200
H	1.77809000	-0.41720500	-2.58049900
H	-2.81016200	0.28246800	-2.22605700
H	-0.97646900	-2.29324600	-3.25491700
H	0.77519700	-1.84519300	-4.42014200
H	0.30141700	-0.37896000	-5.28332000
H	2.43991600	-1.26245300	-6.16681800
H	3.16144200	-1.22191600	-4.55189400
H	2.23735700	1.20963600	-6.18979200
H	3.91224000	0.76289900	-5.83790000
H	3.07428700	2.59926700	-4.31512100
H	3.54893700	1.15795000	-3.40499900
H	0.68777400	1.94646000	-4.17682400
H	1.39835100	2.02830200	-2.55460500
H	-1.71571800	0.34034700	-5.09956800
H	-2.45955300	-1.07768300	-4.34846900
H	-4.58717200	0.15963300	-4.02913100
H	-4.11032000	0.16529800	-5.73339000
H	-4.90060800	2.43583200	-4.96809900
H	-3.22149900	2.47248900	-5.52380900
H	-4.15270600	2.36213200	-2.59197800
H	-3.40685000	3.74689700	-3.40270000
H	-1.76689200	2.49884300	-1.98673600
H	-1.29525500	2.48532200	-3.69742200

H	1.24943100	-2.62067700	-2.13720800
H	0.47200500	-2.61133200	-0.56844400
H	0.87671100	-4.93617300	-1.31835000
H	-0.01310300	-4.65286400	-2.82007600
H	-1.18659600	-4.61100600	0.02088100
H	-1.48224900	-5.84499200	-1.21137500
H	-3.38022000	-4.18183000	-1.06422700
H	-2.62527800	-4.18905400	-2.66289300
H	-2.13417500	-2.13937100	-0.41876000
H	-3.03159700	-1.87024100	-1.90101100
C	0.07094200	-0.08434400	2.44805800
C	-0.43785900	1.19127200	2.61255900
H	-0.56206200	-0.96530300	2.29014100
C	1.39543700	-0.13286200	3.19174200
H	-1.48664600	1.46423700	2.50646600
C	0.56859300	1.96188200	3.43951300
C	1.90086200	1.31391200	3.01837200
C	0.39088300	1.33453300	4.87245000
C	0.97464400	-0.10106300	4.70279100
H	2.08186500	-0.93672100	2.90873400
H	0.49512400	3.05577300	3.41123900
H	2.72664000	1.55815200	3.70312700
H	2.19521500	1.53098900	1.98606300
H	0.96944000	1.92522200	5.59876400
H	1.86177900	-0.25277000	5.33586500
H	-0.65767800	1.33880000	5.20325200
H	0.25010800	-0.88904600	4.95399200

2mCa



Energy: -6602.357054

N	-0.90101400	0.43844200	-0.91171400
C	0.10612300	0.05344500	-0.08617900
N	1.17378100	-0.28570600	-0.85010600
C	0.88052600	-0.20890800	-2.30258300
C	-0.50104000	0.45393000	-2.33726300
C	-2.22558600	0.85514600	-0.51585900
C	2.45814200	-0.78243500	-0.43110000
C	-3.26018100	-0.10689300	-0.48662400
C	-4.53814100	0.31072400	-0.09419800
C	-4.82168800	1.64241800	0.23022000
C	-3.79134800	2.58203100	0.10771100
C	-2.49244100	2.22280000	-0.27876900
C	3.52984500	0.12702900	-0.30409300
C	4.79436000	-0.38459000	0.01678900
C	5.01998100	-1.75375000	0.20008900
C	3.93752300	-2.62774400	0.04058000
C	2.65298300	-2.17471000	-0.28589300
C	-3.03332100	-1.53495200	-0.90520700
H	-5.33807200	-0.43324000	-0.05227300
C	-6.19561800	2.05146500	0.70029400
H	-4.00145100	3.63615100	0.30845400
C	-1.45032800	3.29131900	-0.48276700
C	3.33734500	1.60763900	-0.49841400
H	5.62904300	0.31370400	0.12153800
C	6.38666800	-2.27532500	0.57014500
H	4.09507000	-3.70331900	0.16258600
C	1.52936000	-3.15841200	-0.48050900
H	-3.95152300	-2.12339500	-0.77490000
H	-2.24200800	-2.00495000	-0.30533900
H	-2.74808600	-1.59902600	-1.96828200
H	-6.24666800	2.05486800	1.80188100
H	-6.96741800	1.35663000	0.34012900
H	-6.45848600	3.06343600	0.35944000
H	-1.83695900	4.26999900	-0.16745100
H	-1.17484200	3.37722800	-1.54693600
H	-0.53660900	3.09095400	0.09408800
H	4.28377600	2.14370400	-0.34372500
H	2.59457600	2.00680300	0.20952000
H	2.98566000	1.84674200	-1.51505700
H	6.46313000	-2.44440100	1.65705600
H	7.17753300	-1.56499000	0.29117500
H	6.59838000	-3.23418800	0.07472400
H	1.86651600	-4.17946200	-0.25468300
H	1.16608800	-3.15697700	-1.52125400
H	0.67014300	-2.93128700	0.16877600
H	0.87524100	-1.22071900	-2.73491200
H	-1.22623300	-0.10338800	-2.94414600
H	1.65148700	0.38021600	-2.81578000

H	-0.46386100	1.49024400	-2.70529300
Ru	-0.08479400	0.07662000	1.97486800
Cl	-1.08606000	-2.15200200	1.90303400
Cl	0.80123800	2.36532800	2.03843200
C	1.54850200	-0.63269600	2.43942200
H	2.42144000	0.01119100	2.62726800
H	1.67737200	-1.71370700	2.60364500
C	-0.16548200	0.66947400	4.53184800
C	-1.39739600	0.49258600	3.93655300
C	-0.10371900	-0.27259600	5.71461200
H	0.47179900	1.54273600	4.40004300
C	-2.13527700	-0.55552200	4.75303200
H	-1.90188900	1.26919700	3.35086900
C	-0.97118900	-1.44920500	5.22944000
C	-1.08450500	0.39695800	6.74766900
C	-2.48226400	0.19091400	6.08916000
H	0.89264400	-0.49810000	6.11377800
H	-2.97606400	-1.05252600	4.25859500
H	-1.26473200	-2.12652100	6.04546200
H	-0.52336700	-2.02056500	4.40945800
H	-0.84387000	1.45465900	6.92690000
H	-1.00860500	-0.12749400	7.71226100
H	-3.01578800	1.13604800	5.91327500
H	-3.12952800	-0.44444700	6.71243700

1mCi (Ru-norbornene at 20Å taken as the reference state for binding energy)

Energy: -6724.0892352

C	-0.20246200	1.92121200	0.37869300
Cl	2.05143000	-0.53142000	0.54505100
Ru	-0.20323100	0.08531200	0.41216700
Cl	-2.34390900	-0.54953500	1.11272100
H	-0.06592900	2.39260400	1.37152500
H	-0.31493700	2.61494800	-0.46284000
P	-0.51623200	-0.36011700	-1.81819400
C	0.96289500	0.17024900	-2.86775400
C	-2.14835000	0.27832100	-2.50859000
C	-0.63173800	-2.21945100	-2.13308200
C	1.12064400	-0.48883700	-4.25651600
C	2.46177100	-0.09559500	-4.90153000
C	2.62174900	1.42494800	-5.00780200
C	2.44404400	2.08800800	-3.63796400
C	1.10704400	1.70159900	-2.98502000
C	-2.39326000	-0.01774200	-4.00342800
C	-3.84360300	0.31355000	-4.39796000
C	-4.19147000	1.77158400	-4.07674800
C	-3.92324200	2.08526100	-2.60060900
C	-2.47957400	1.74964700	-2.18881400
C	0.60728100	-2.97903600	-1.61539900
C	0.55754900	-4.46424900	-2.00826800
C	-0.72811700	-5.13564600	-1.51345700
C	-1.96635400	-4.37542800	-1.99998500
C	-1.92272400	-2.88597800	-1.61444700
H	1.79521400	-0.17755000	-2.23200900
H	-2.86026300	-0.32147900	-1.91663600
H	-0.64162400	-2.30344100	-3.23335200
H	1.07158700	-1.58356700	-4.18205800
H	0.30102700	-0.17679400	-4.92128900
H	2.53555800	-0.56210900	-5.89780000
H	3.28827600	-0.51055900	-4.29835200
H	1.86734600	1.82254000	-5.71062100
H	3.60754200	1.67723700	-5.43146900
H	2.50377900	3.18480600	-3.73026700
H	3.26849900	1.78336600	-2.97081400
H	0.28110700	2.11030800	-3.59022100
H	1.04690700	2.16245800	-1.99108100
H	-1.71453000	0.59765200	-4.61499700
H	-2.17694600	-1.06846400	-4.24463400
H	-4.52971000	-0.35768100	-3.85197600
H	-3.98792200	0.10796100	-5.47148500
H	-5.24409500	1.97910400	-4.32821600
H	-3.57936500	2.43752100	-4.71142900
H	-4.61575000	1.50076300	-1.97028300
H	-4.12744900	3.14735400	-2.38857400
H	-2.36091400	1.92857000	-1.11253200
H	-1.78606100	2.42200900	-2.71950400
H	1.53651400	-2.52765500	-1.98989600
H	0.65545000	-2.89542200	-0.51905000
H	1.44212100	-4.97633000	-1.59606000
H	0.62264200	-4.55832400	-3.10757000
H	-0.72467900	-5.15790600	-0.40964900
H	-0.76657600	-6.18477900	-1.84954700
H	-2.88197600	-4.82695600	-1.58466700
H	-2.04288600	-4.46692800	-3.09885600
H	-1.98317000	-2.77967000	-0.52130500
H	-2.81347400	-2.39029900	-2.02446700
C	0.28576700	-1.31781900	20.30677100
C	-0.33182300	-0.13347300	20.47836100
H	-0.13242200	-2.22064700	19.85873500
C	1.62224100	-1.24344700	21.02827500
H	-1.35392800	0.12584400	20.19752500
C	0.58880800	0.74363800	21.31356900

C	1.96685200	0.24905600	20.81543900
C	0.57921300	0.13475600	22.75990000
C	1.28237500	-1.24237300	22.56094800
H	2.37821000	-1.98163300	20.73005600
H	0.39943800	1.82416100	21.27632600
H	2.80707100	0.59717700	21.43711000
H	2.15307200	0.49576800	19.76040300
H	-0.44071600	0.04433100	23.15901200
H	1.15134800	0.77935100	23.44515000
H	0.64341400	-2.09333200	22.83469100
H	2.20512700	-1.31269000	23.15781200

2mCi (Ru-norbornene at 20Å taken as the reference state for binding energy)

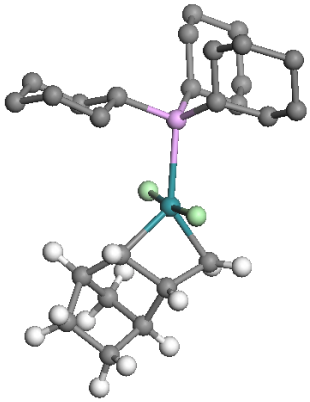
Energy: -6602.3515757

N	-0.86496900	0.44898000	-0.88784500
C	0.14297400	0.06513300	-0.04569500
N	1.20962700	-0.27929100	-0.82425900
C	0.90867200	-0.20943400	-2.27341200
C	-0.45450100	0.48400300	-2.30566400
C	-2.19875900	0.85417600	-0.52142400
C	2.49591300	-0.79484600	-0.44613900
C	-3.21399700	-0.12671700	-0.47361800
C	-4.50325000	0.27498700	-0.10945100
C	-4.81330600	1.60978800	0.17951900
C	-3.80213900	2.56572100	0.03748200
C	-2.49352600	2.22034800	-0.32750600
C	3.56901100	0.10406100	-0.28864700
C	4.84005800	-0.42700300	-0.02946500
C	5.06462500	-1.80499200	0.07666100
C	3.97039900	-2.66633300	-0.07812700
C	2.67969500	-2.18969600	-0.34168400
C	-2.95704100	-1.55849000	-0.86757200
H	-5.28858400	-0.48290100	-0.04812400
C	-6.19380500	2.00128100	0.64373300
H	-4.03139200	3.61919700	0.21899600
C	-1.48327500	3.31128200	-0.57528100
C	3.36365000	1.59472100	-0.37203700
H	5.67995800	0.26161800	0.09489400
C	6.44056600	-2.34615500	0.37931900
H	4.12200200	-3.74588000	0.00899400
C	1.52557200	-3.15118000	-0.47929100
H	-3.81303800	-2.19083600	-0.59874900
H	-2.07233800	-1.97112600	-0.36995300
H	-2.81361400	-1.64680300	-1.95838800
H	-6.24666100	1.99849500	1.74509900
H	-6.95655800	1.29885200	0.27871300
H	-6.46674700	3.01161400	0.30631000
H	-1.69843800	4.18979800	0.04699700
H	-1.52551800	3.63851300	-1.62881800
H	-0.46016400	2.99643000	-0.34656700
H	4.30707400	2.12762000	-0.19232200
H	2.62832600	1.93880000	0.37014100
H	2.99345700	1.90301800	-1.36271800
H	6.56732400	-2.51822800	1.46109100
H	7.22545900	-1.64475600	0.06374200
H	6.61579300	-3.30559900	-0.12813200
H	1.83996700	-4.17266800	-0.22648000
H	1.13136900	-3.17468500	-1.50792900
H	0.69332600	-2.87893300	0.18491800
H	0.87790400	-1.22446200	-2.69902500
H	-1.18812000	-0.04427600	-2.92856900
H	1.69293900	0.35563100	-2.79441300
H	-0.39193600	1.52679600	-2.65411000
Ru	-0.07334600	0.13019600	1.93984700
Cl	-1.57590100	-1.63755700	2.28926300
Cl	0.27552100	2.43440700	2.23204100
C	1.50485300	-0.58202800	2.54309500
H	1.61158700	-0.58944200	3.64583500
H	2.33436300	-1.01517200	1.97565900
C	-5.33719100	4.34955400	20.86269000
C	-6.54512700	4.17876700	20.29149000
C	-5.26827100	3.42402700	22.06737400
H	-4.58640000	5.09893500	20.60604000
C	-7.29346100	3.13750100	21.10941200
H	-6.97826100	4.75901400	19.47498500
C	-6.11574000	2.23739100	21.55162100
C	-6.25034500	4.02735100	23.13225600
C	-7.64889600	3.82952100	22.47299300

H	-4.26517500	3.19571900	22.45097400
H	-8.14279700	2.64740300	20.61574300
H	-6.38816800	1.51631900	22.33885100
H	-5.64161500	1.71336700	20.70922700
H	-6.02204000	5.08082700	23.34577300
H	-6.17101000	3.47073900	24.07908300
H	-8.18958000	4.77399000	22.32073300
H	-8.28956600	3.17214100	23.08104700

Stage D

1mD

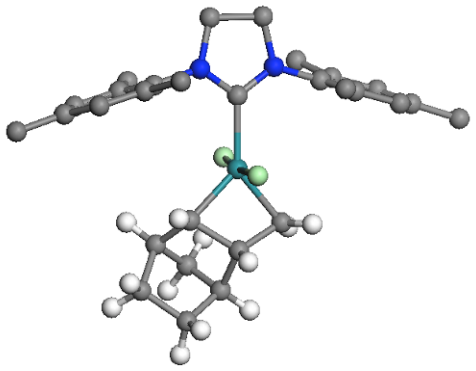


Energy: -6724.105479

C	0.59121900	-0.67591000	3.26516500
C	0.70669100	2.01465700	2.98280000
Ru	0.27390700	0.52318400	1.69064300
Cl	-2.08117700	0.58406700	2.27332500
Cl	2.60968400	0.55443300	0.92448500
P	-0.26130900	0.19283600	-0.70168900
C	0.98139000	0.89921500	-1.91009200
C	-0.26119600	-1.65876100	-1.02551600
C	-2.01172500	0.74555500	-1.09114900
C	-2.22213400	2.26491700	-0.92094100
C	-3.72045200	2.60465300	-0.95544500
C	-4.38245300	2.10445900	-2.24574100
C	-4.13438500	0.60476800	-2.45345900
C	-2.63325800	0.26245000	-2.41770400
C	1.21755800	2.41574100	-1.74452900
C	2.44203300	2.85218300	-2.56592100
C	2.29983200	2.47710900	-4.04652900
C	2.00742500	0.98121200	-4.21803100
C	0.78094800	0.54277500	-3.39657600
C	1.13711500	-2.29553900	-0.88278300
C	1.09738800	-3.79424600	-1.22159800
C	0.06874500	-4.54669600	-0.37036300
C	-1.31892200	-3.90758300	-0.49964300
C	-1.29161900	-2.40974200	-0.15526600
H	1.90524100	0.41543300	-1.55438700
H	-0.57305300	-1.75840700	-2.08010800
H	-2.56111500	0.27269700	-0.26037900
H	-1.78910500	2.60611100	0.02995600
H	-1.71415300	2.80601000	-1.73443000
H	-3.85378000	3.69431000	-0.85378800
H	-4.20815800	2.14298800	-0.08075800
H	-3.97090300	2.66164300	-3.10711300
H	-5.46482500	2.31078900	-2.22781400
H	-4.56244600	0.27226600	-3.41348500
H	-4.65235600	0.03588200	-1.66187900
H	-2.13665300	0.74956200	-3.27072400
H	-2.50429200	-0.82232700	-2.54994700
H	0.33526300	2.97830000	-2.08729200
H	1.37948000	2.65683500	-0.68475900
H	3.33979800	2.37167600	-2.14182500
H	2.58679200	3.94001700	-2.45949800
H	3.21237000	2.74906300	-4.60202200
H	1.47463800	3.06001300	-4.49419900

H	2.88581600	0.39581300	-3.89388900
H	1.84346600	0.73975500	-5.28140000
H	0.61937700	-0.53758500	-3.53253600
H	-0.11175500	1.05194300	-3.79191500
H	1.86427200	-1.79363600	-1.53529700
H	1.50344400	-2.15135300	0.14460100
H	2.10218800	-4.22533700	-1.08349600
H	0.84772500	-3.92165400	-2.29074900
H	0.38413000	-4.52427400	0.68749300
H	0.03154500	-5.60793000	-0.66505400
H	-2.04266000	-4.41832000	0.15603000
H	-1.68687700	-4.03742000	-1.53362300
H	-1.03498000	-2.28142600	0.90819800
H	-2.29717800	-1.98396600	-0.27741500
H	1.71556400	2.43041800	2.89121200
H	-0.09686500	2.75083700	3.09179300
C	0.57209400	0.81335500	3.95424600
H	-0.34543700	-1.21209000	3.46560900
C	1.83747400	-1.33891100	3.84069000
C	1.78411100	0.64352900	4.92538400
H	-0.40320900	0.90019000	4.44922700
C	2.80357900	-0.17633000	4.12367400
C	1.35712200	-0.36597900	6.02233300
C	1.43363900	-1.74299200	5.29170900
H	2.22091800	-2.16855700	3.23343200
H	2.12771200	1.61047100	5.31602900
H	3.16345500	0.31257100	3.21416800
H	3.66031100	-0.48418500	4.74363500
H	0.35819800	-0.14823600	6.42787400
H	2.06712900	-0.31935700	6.86147100
H	0.48581700	-2.30002000	5.32927500
H	2.21182800	-2.38792400	5.72829700

2mD



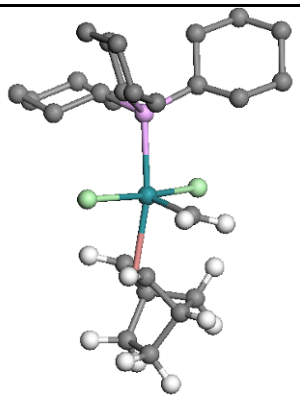
Energy: -6602.377330

N	-0.94693500	0.35648900	-0.70347200
C	0.11314900	-0.04095200	0.03401400
N	1.15360900	-0.30167600	-0.78745300
C	0.83942800	0.02632700	-2.20109800
C	-0.67045700	0.28531400	-2.16044400
C	-2.25571200	0.73847900	-0.22564200
C	2.47638600	-0.75788600	-0.42704800
C	-3.26460500	-0.23944300	-0.09236900
C	-4.52761100	0.18018700	0.34600100
C	-4.81627200	1.51995500	0.62703800
C	-3.80562100	2.46721300	0.42645000
C	-2.52409200	2.10738800	-0.00940500
C	3.46859600	0.18368800	-0.08033600
C	4.74232500	-0.29718200	0.25161000
C	5.06053400	-1.65890600	0.21392600
C	4.07082600	-2.55202300	-0.21239300
C	2.77910300	-2.13145400	-0.54942700
C	-3.03142700	-1.68930400	-0.42405700
H	-5.31389300	-0.57116400	0.45943800
C	-6.17534700	1.92871000	1.13872400
H	-4.01806700	3.52432100	0.60748600
C	-1.48306900	3.17042000	-0.24218700
C	3.21082000	1.66764300	-0.09210400
H	5.51112100	0.42478900	0.54032500
C	6.42507100	-2.15399500	0.62386800
H	4.30810800	-3.61643400	-0.28934400
C	1.77583100	-3.12876700	-1.06650600
H	-3.93905600	-2.27738900	-0.22973500
H	-2.21020700	-2.11661700	0.17098900
H	-2.77799100	-1.82528200	-1.48788200
H	-6.18664200	1.95567900	2.24103500
H	-6.95451600	1.22206800	0.81973300
H	-6.45762300	2.93158900	0.78665800
H	-1.92221300	4.16996400	-0.11965400
H	-1.06125200	3.11691900	-1.25818400
H	-0.65040300	3.07148700	0.47071200
H	4.13615600	2.21834200	0.12702800
H	2.45547600	1.96394200	0.65095800
H	2.85518100	2.00661100	-1.07800600
H	6.43134800	-2.44451600	1.68755900
H	7.19498400	-1.38057600	0.49110200
H	6.72303800	-3.03927400	0.04354100
H	2.13990300	-4.15420800	-0.91782200
H	1.60406600	-2.99818900	-2.14885000
H	0.81462600	-3.03244000	-0.54520400
H	1.11382200	-0.81018700	-2.85526700
H	-1.25104600	-0.53392700	-2.61000100
H	1.41302400	0.91312500	-2.51011100

H	-0.95906800	1.22448300	-2.64901900
Ru	0.11124000	-0.16384900	2.11639000
Cl	-0.29249100	-2.54566900	1.69637200
Cl	0.70677400	2.18113600	2.39228800
C	1.36377700	-0.67991600	3.61798700
H	2.25311300	-0.04570800	3.68688300
H	1.54627000	-1.75570600	3.70499900
C	0.15618600	-0.14024000	4.43074600
C	-1.23165100	0.06349300	3.58767600
C	-0.36607100	-1.11294000	5.53282000
H	0.43339500	0.85724400	4.79482000
C	-2.21377500	-0.89946900	4.24494800
H	-1.54855300	1.11350500	3.58301000
C	-1.33776700	-2.04040600	4.78887900
C	-1.33151300	-0.30515900	6.43884600
C	-2.62578400	-0.19177500	5.57215600
H	0.45855400	-1.59665900	6.07372100
H	-3.05783800	-1.17857900	3.60238900
H	-1.89000400	-2.69820900	5.47887700
H	-0.87491600	-2.63982700	3.99998900
H	-0.91918500	0.67437200	6.72319300
H	-1.51962600	-0.86122500	7.36979300
H	-2.94456100	0.84899900	5.41495000
H	-3.46852000	-0.72801800	6.03572900

Transition State TS-CD

1mTS-CD

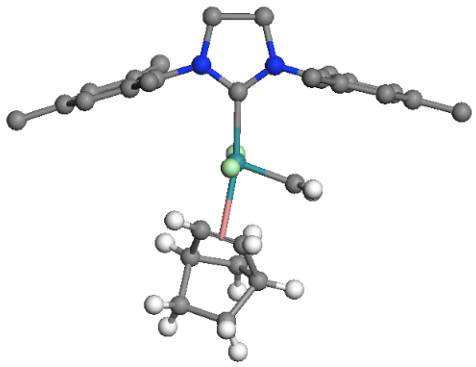


Energy: -6724.087582
Imaginary Frequency: 215i cm^{-1}

C	0.15310500	2.03640200	0.48590400
Cl	2.07625300	-0.48248900	-0.01599400
Ru	-0.24618300	0.24366600	0.21421700
Cl	-2.66324000	0.59737900	0.39254100
H	-0.62712900	2.81310500	0.52056600
H	1.19124400	2.37569800	0.62632600
P	-0.49046900	-0.15823100	-2.19187700
C	1.07422300	0.15512600	-3.17525500
C	-1.97899200	0.72214000	-2.92528900
C	-0.85912300	-1.98451200	-2.46765300
C	1.08419700	-0.30844700	-4.64629500
C	2.50921100	-0.22134400	-5.22168600
C	3.08782500	1.19342100	-5.09322200
C	3.02787700	1.68960200	-3.64260900
C	1.60457100	1.59874400	-3.06929900
C	-2.43692200	0.28937500	-4.33333100
C	-3.78800600	0.94081500	-4.68135400
C	-3.72536000	2.46938800	-4.57605500
C	-3.23116800	2.90652500	-3.19149300
C	-1.88174800	2.25869800	-2.84345600
C	0.32637800	-2.90926800	-2.12121100
C	-0.01058000	-4.37747300	-2.43112100
C	-1.28344900	-4.83664600	-1.71097100
C	-2.46120600	-3.90991600	-2.03318900
C	-2.13289200	-2.44038800	-1.72404100
H	1.78726700	-0.46572000	-2.60749600
H	-2.75900700	0.43086100	-2.20196900
H	-1.05016300	-2.08142700	-3.55041000
H	0.71128200	-1.33857200	-4.74511900
H	0.41902200	0.33084600	-5.24773500
H	2.50159700	-0.54040300	-6.27718800
H	3.15825200	-0.93275600	-4.68144500
H	2.50819900	1.87909600	-5.73765400
H	4.12576700	1.21515300	-5.46429500
H	3.38626400	2.73055500	-3.58131900
H	3.70195900	1.08387400	-3.01349800
H	0.94964600	2.28380800	-3.63026600
H	1.60477200	1.92351300	-2.01977200
H	-1.69122800	0.59451600	-5.08382400
H	-2.53397600	-0.80365100	-4.40543100
H	-4.55966100	0.55934400	-3.98989800
H	-4.09355400	0.63523000	-5.69596700
H	-4.71468400	2.90752100	-4.78731700

H	-3.03716100	2.85839500	-5.34844100
H	-3.97122100	2.61967400	-2.42528800
H	-3.13668500	4.00400200	-3.14554900
H	-1.57277400	2.56328900	-1.83430300
H	-1.11896800	2.62451000	-3.54877100
H	1.22763200	-2.61874400	-2.67814500
H	0.58418300	-2.80160600	-1.05643500
H	0.84345700	-5.01392700	-2.14781100
H	-0.14355000	-4.50015400	-3.52170800
H	-1.10601600	-4.83296900	-0.62095500
H	-1.52791900	-5.87578900	-1.98578600
H	-3.35670500	-4.20919100	-1.46429600
H	-2.72231700	-4.00786700	-3.10263100
H	-1.99093500	-2.31826900	-0.63791400
H	-2.99167400	-1.80651300	-1.98371500
C	-0.25080200	-0.38379800	2.39224500
C	-0.42513700	1.00768700	2.55452100
H	-1.12084900	-1.04203400	2.29878400
C	0.95677600	-0.76296100	3.23737900
H	-1.40556600	1.48074300	2.50483400
C	0.67080100	1.47071200	3.49929500
C	1.82487500	0.51009700	3.16840100
C	0.19661700	0.88472900	4.87837900
C	0.41250900	-0.65008300	4.70351200
H	1.44410500	-1.71212700	2.99128700
H	0.88360000	2.54614400	3.51526300
H	2.61167100	0.52138700	3.93739700
H	2.26988700	0.66098400	2.18016500
H	0.83036000	1.29430600	5.67936400
H	1.16591900	-1.03061700	5.40974300
H	-0.84398800	1.15048200	5.11317900
H	-0.50855100	-1.23073200	4.85676000

2mTS-CD



Energy: -6602.355957
Imaginary Frequency: 231i cm^{-1}

N	-1.01783356	0.37626977	-0.88528362
C	-0.00361677	0.03068888	-0.05585341
N	1.08861111	-0.24488944	-0.80663930
C	0.82236277	-0.13622173	-2.26215053
C	-0.61522277	0.39344692	-2.31104495
C	-2.35314647	0.77237227	-0.50598215
C	2.40196312	-0.64929460	-0.37427491
C	-3.38643952	-0.18936084	-0.52258270
C	-4.67548186	0.22219058	-0.16020448
C	-4.96940907	1.54762600	0.17720971
C	-3.93527226	2.48749395	0.10479331
C	-2.62599197	2.13411561	-0.24612677
C	3.39425814	0.33764906	-0.20043228
C	4.68399982	-0.07936217	0.15256201
C	5.00952632	-1.42928711	0.32325497
C	4.00619159	-2.38144003	0.11077154
C	2.69992290	-2.02262092	-0.24863476
C	-3.15281884	-1.61018766	-0.96112635
H	-5.47526215	-0.52253086	-0.15194784
C	-6.35718556	1.95251043	0.60704549
H	-4.15075459	3.53728863	0.31989476
C	-1.57488061	3.20319921	-0.38840608
C	3.09786420	1.80295261	-0.37749070
H	5.45780197	0.67982478	0.29308981
C	6.39855283	-1.84516999	0.74087191
H	4.24378295	-3.44279442	0.21993440
C	1.66529041	-3.08808194	-0.49710342
H	-4.04499057	-2.22136199	-0.77153380
H	-2.31040221	-2.06543183	-0.42435851
H	-2.94678233	-1.66237404	-2.04316622
H	-6.43223003	1.98582633	1.70635351
H	-7.11430834	1.24154925	0.24831366
H	-6.62205533	2.95262355	0.23435494
H	-1.98709698	4.18502268	-0.11975238
H	-1.21453110	3.27125930	-1.42763293
H	-0.70744440	3.01426792	0.25898253
H	4.00606357	2.40006136	-0.21855952
H	2.33399931	2.14185382	0.33838279
H	2.72800909	2.02964921	-1.38995491
H	6.47687234	-1.90733807	1.83880929
H	7.15439702	-1.12381977	0.40005784
H	6.66362944	-2.83367579	0.33954182
H	2.07401697	-4.08245382	-0.27159601
H	1.34188732	-3.09906556	-1.55060480
H	0.76781599	-2.93707042	0.12085746
H	0.92744545	-1.12286281	-2.73552354
H	-1.28351799	-0.24424724	-2.90398412

H	1.54569092	0.54614859	-2.72761234
H	-0.67541292	1.41812045	-2.70545412
Ru	-0.15582277	-0.05499431	2.02980262
Cl	-1.08201819	-2.29882240	1.75531140
Cl	0.59845611	2.27084200	2.22681651
C	1.44730221	-0.68821683	2.71575798
H	2.30154358	-0.02322310	2.90792411
H	1.58328166	-1.75522835	2.94532758
C	0.08249649	0.17286874	4.49464691
C	-1.24025108	0.23154489	4.01433607
C	0.10496471	-0.90166622	5.56779536
H	0.73407637	1.04539658	4.51758171
C	-2.02096568	-0.81880842	4.79102234
H	-1.68792209	1.18585295	3.72175570
C	-0.95123246	-1.89625023	5.06118634
C	-0.67945342	-0.22270636	6.74660573
C	-2.14635190	-0.18586732	6.21990688
H	1.08965324	-1.29381921	5.84864199
H	-2.96327867	-1.15210434	4.34481507
H	-1.26409576	-2.60915496	5.83855025
H	-0.66264180	-2.43722255	4.15516857
H	-0.28562403	0.77371064	6.99316205
H	-0.58736986	-0.84575515	7.64872054
H	-2.56568915	0.83000312	6.19463285
H	-2.80994696	-0.80497824	6.84186805

Structures for cis/trans isomer for 1C and 1D by BP86/DND

Cartesian coordinates in angstroms and energies in hartrees

cis- 1Ca

Energy: -6955.194765			
C	0.30873500	2.23138800	0.10095500
Cl	2.21111100	-0.67228200	0.05435300
Ru	-0.00616900	0.36713400	0.22347300
Cl	-2.42292200	0.76160300	0.44945600
H	-0.62504300	2.81016400	0.21321800
C	1.47091600	3.09983000	-0.00641000
P	-0.38382700	-2.35415100	0.00000000
C	1.13645100	-0.18243600	-3.20318100
C	-1.83709900	0.62788500	-2.89984400
C	-0.90093900	-4.21897600	0.00000000
C	1.13668700	-1.05193500	-4.47852100
C	2.52054000	-1.02043600	-5.15341800
C	2.97245200	0.41014500	-5.47019400
C	2.93213300	1.29261500	-4.21639700
C	1.54559200	1.26238800	-3.55355900
C	-2.22655500	0.18260400	-4.32427500
C	-3.57595400	0.80303600	-4.73122000
C	-3.55284800	2.33288700	-4.62573900
C	-3.11724200	2.78397200	-3.22625200
C	-1.76840700	2.16588300	-2.82585400
C	0.19903500	-3.03546700	-1.65309800
C	-0.23081000	-6.33683700	0.00000000
C	-1.55502000	-5.91792000	0.00000000
C	-2.64993100	-5.39696100	0.00000000
C	-2.22316600	-3.75768100	0.00000000
H	1.90596600	-0.57582200	-2.51662900
H	-2.64692700	0.33771800	-2.21067300
H	-1.07097300	-5.49818300	0.00000000
H	0.87636900	-2.09453100	-4.25131000
H	0.38186600	-0.68274800	-5.19088300
H	2.49387500	-1.62866500	-6.07308500
H	3.25753300	-1.49561700	-4.48239700
H	2.30567000	0.83987000	-6.23969600
H	3.98671200	0.40244700	-5.90229800
H	3.19745400	2.33180200	-4.47056900
H	3.68597000	0.94118000	-3.49129600
H	0.81285900	1.69279000	-4.25498700
H	1.54421800	1.89452600	-2.65536800
H	-1.45519600	0.50890800	-5.04055200
H	-2.29220200	-5.31477500	0.00000000
H	-4.36633800	0.40373300	-4.07149600
H	-3.83343000	0.49116200	-5.75716400
H	-4.54439900	2.74674100	-4.87335700
H	-2.84705300	2.73655500	-5.37435200
H	-3.87843400	2.48487200	-2.48541900
H	-3.04714500	3.88347600	-3.18190500
H	-1.50907500	2.47742600	-1.80686300
H	-0.98539800	2.54705500	-3.49891500
H	1.14904600	-2.85772200	-2.17428900
H	0.40825800	-2.84469300	-0.58949000
H	0.56461400	-5.16506800	-1.46402200
H	-0.33979800	-7.63256800	0.00000000
H	-1.40844800	-4.72947800	0.00000000
H	-1.86644900	-7.14282100	0.00000000
H	-3.57909100	-5.00654900	0.00000000
H	-2.88981300	-6.64805200	0.00000000
H	-2.10275100	-2.45937200	0.00000000
H	-3.02650200	-3.45512700	0.00000000
C	0.03098600	-0.18835500	2.52088800

C	-0.20136900	1.17093000	2.65296300
H	-0.77647000	1.45422700	0.00000000
C	1.28190300	-0.49563200	3.32800300
H	-1.17039800	1.64816200	2.51709400
C	0.91412600	1.73313900	3.50464700
C	2.09103700	0.80465900	3.15357100
C	0.55344800	1.19760300	4.94007900
C	0.80702400	-0.33601100	4.81498000
H	1.79336600	-1.43509600	3.09519700
H	1.07861700	2.81573400	3.45042200
H	2.92304400	0.88620700	3.86866300
H	2.46337800	0.92837200	2.13276100
H	1.22689200	1.65971100	5.67773300
H	1.60031100	-0.66939800	5.50066600
H	-0.47743600	1.44453300	5.23156300
H	-0.09012400	4.09619300	0.00000000
C	1.24322200	4.49990300	0.06075800
C	2.29466800	5.40870200	-0.03112200
C	3.60439400	4.94238600	-0.19079200
C	3.85089800	3.56503700	-0.26351500
C	2.80261300	2.65301300	-0.17635000
H	0.22061500	4.86356600	0.18426700
H	2.09608500	6.48102000	0.02306300
H	4.43208900	5.65162200	-0.25985000
H	4.87282300	3.20077500	-0.38760500
H	2.98779800	1.57960800	-0.23218900

trans- 1Ca

Energy: -6955.196817

C	-0.03798900	2.24368300	-0.04067700
Cl	2.04273400	-0.09016900	-0.04368800
Ru	-0.33818800	0.40198000	0.23926600
Cl	-2.74560100	0.12262200	0.51658600
C	-0.75207300	3.45595100	0.32933000
H	0.91401700	2.45562400	-0.55346000
P	-0.64944700	-2.33218900	0.00000000
C	0.85908900	0.10945100	-3.17688400
C	-2.20943500	0.41296400	-2.92505700
C	-0.85791700	-4.31099700	0.00000000
C	1.11105100	-0.78094900	-4.41162700
C	2.50890000	-0.49787600	-4.99333000
C	2.70660900	0.98345200	-5.33440500
C	2.39686200	1.87898800	-4.12969300
C	0.99586000	1.59440200	-3.56657400
C	-2.41877700	-4.43313000	0.00000000
C	-3.80647400	0.35925600	-4.90111900
C	-4.03593600	1.86869500	-4.76764000
C	-3.80443900	2.33674500	-3.32649200
C	-2.41438100	1.93551600	-2.80796600
C	0.28085100	-2.85091700	-1.47419500
C	0.17581500	-4.37053500	-1.67315200
C	-1.18677800	-6.12875200	0.00000000
C	-2.32463500	-6.08738200	0.00000000
C	-2.22586100	-4.36667700	0.00000000
H	1.66316200	-0.09732600	-2.45082400
H	-2.99090500	-2.33660600	0.00000000
H	-0.77570200	-5.61541200	0.00000000
H	1.05084600	-1.84647500	-4.15292000
H	0.34976600	-0.59526500	-5.18591500
H	2.66780900	-1.12000200	-5.88933400
H	3.26848700	-0.80771500	-4.25533900
H	2.03879800	1.25685200	-6.17082500
H	3.73638400	1.15803900	-5.68611100
H	2.47363500	2.94150500	-4.41332400
H	3.14304900	1.70627400	-3.33581500
H	0.24477100	1.85513200	-4.32975000
H	0.80714900	2.24160100	-2.70037000
H	-1.65119800	0.40186700	-5.02616200
H	-2.30350000	-5.61449700	0.00000000
H	-4.58304700	-4.51196700	0.00000000
H	-3.91163000	0.04389800	-5.95232600
H	-5.05443900	2.13124200	-5.09724900
H	-3.34198400	2.40390200	-5.44059900
H	-4.57240400	1.89605600	-2.66770300
H	-3.92086800	3.43023800	-3.25488800
H	-2.30951200	2.24315800	-1.76106000
H	-1.64747600	2.47299100	-3.38530300
H	1.26572800	-2.49346100	-1.80254000
H	0.23193300	-2.62312600	-0.39746000
H	0.99091800	-4.86831500	-1.12367900
H	0.32772800	-4.60997800	-2.74108000
H	-1.28693700	-4.90575800	0.00000000
H	-1.25904300	-7.40536200	0.00000000
H	-3.30260100	-6.07031900	0.00000000
H	-2.29659700	-7.39864000	0.00000000
H	-2.37528500	-3.05711700	0.00000000
H	-3.04726200	-4.42680200	0.00000000
C	0.03272700	-0.19426700	2.53125100
C	-0.55979400	1.03822300	2.70419700
H	-0.52584400	1.25345100	0.00000000
C	1.37897900	-0.13924400	3.23171800
H	-1.62779400	1.23324600	2.64626200

C	0.42009700	1.89689000	3.47805800
C	1.77850800	1.33464000	3.01888800
C	0.35497400	1.29658300	4.92968200
C	1.00168400	-0.11124500	4.75503100
H	2.10900400	-0.90032300	2.93979800
H	0.27141600	2.98155100	3.42639800
H	2.60756700	1.64391600	3.67247700
H	2.02422100	1.55521400	1.97560100
H	0.94699400	1.92963000	5.60776800
H	1.91095200	-0.21720900	5.36547200
H	-0.67108600	1.25779000	5.32154200
H	0.32116100	-0.92922700	5.03056900
C	-0.09072000	4.69645200	0.14006300
C	-0.71861400	5.90365000	0.43637400
C	-2.03299500	5.90695900	0.91459900
C	-2.70825300	4.69375800	1.09877200
C	-2.07871000	3.48464700	0.82071400
H	0.93109200	4.69724500	-0.24615800
H	-0.18707700	6.84488000	0.28451500
H	-2.53377800	6.85175200	1.13494300
H	-3.73697800	4.69309100	1.46547600
H	-2.61055300	2.54179700	0.94962500

cis- 1D

Energy: -6955.194721

C	9.91004100	-1.89066800	3.24212900
C	9.71390200	0.85402900	2.98088300
Ru	9.57990000	-0.68057200	1.64740000
Cl	7.21840600	-0.73980000	2.32763300
Cl	11.82936700	-0.97533200	0.71974900
P	8.81873800	-0.89916300	-0.70533500
C	10.06744900	-0.33500800	-1.98642400
C	8.51688700	-2.71215800	-1.10008900
C	7.15375100	-0.06991000	-0.94409700
C	7.16891700	1.43704800	-0.61284200
C	5.73391100	1.98144300	-0.53547400
C	4.95744800	1.70981900	-1.82986700
C	4.97841300	0.21905200	-2.19206600
C	6.41670200	-0.32411500	-2.27429400
C	10.48464500	1.14136900	-1.82323300
C	11.70719100	1.45251600	-2.70153300
C	11.44467200	1.11926700	-4.17571700
C	10.97683500	-0.33154500	-4.34475100
C	9.75325900	-0.64663000	-3.46383600
C	9.80453200	-3.55823400	-1.01239800
C	9.53690900	-5.01550600	-1.42386800
C	8.41505000	-5.64617800	-0.59102200
C	7.13897500	-4.79963200	-0.66280700
C	7.39641200	-3.34209900	-0.24724800
H	10.94702000	-0.92845400	-1.68932500
H	8.18106900	-2.71688300	-2.15213800
H	6.57956500	-0.54646300	-0.13298200
H	7.68374800	1.60942400	0.34306300
H	7.72044000	1.98910800	-1.38928900
H	5.76068500	3.06315000	-0.32560900
H	5.21962300	1.50523800	0.31624500
H	5.41199100	2.28678800	-2.65583400
H	3.91771500	2.06433300	-1.73717600
H	4.46403400	0.04993900	-3.15257400
H	4.41965100	-0.35161800	-1.42989900
H	6.93893900	0.18040300	-3.10157200
H	6.39043000	-1.39593300	-2.52063900
H	9.65611600	1.80284200	-2.12010100
H	10.72053000	1.35521500	-0.77157300
H	12.56671900	0.86727300	-2.33292300
H	11.97822200	2.51513900	-2.59113800
H	12.35201400	1.29683600	-4.77621500
H	10.66938400	1.80086300	-4.57030300
H	11.80038300	-1.01492500	-4.07274300
H	10.73248000	-0.53766400	-5.40012000
H	9.46943100	-1.70051800	-3.60110500
H	8.90270300	-0.03840500	-3.80713800
H	10.59752700	-3.13665900	-1.64533400
H	10.19190000	-3.52967300	0.01790900
H	10.46719600	-5.59778400	-1.32106200
H	9.26111400	-5.04942900	-2.49342700
H	8.74278800	-5.72007500	0.46111900
H	8.21281200	-6.67495800	-0.93142000
H	6.35478200	-5.22725400	-0.01699100
H	6.74306300	-4.82210100	-1.69454800
H	7.67680500	-3.30212400	0.81601900
H	6.46501700	-2.76646900	-0.33558500
C	10.67107900	1.99071100	2.97569200
H	8.69996500	1.22187700	3.16950100
C	9.90889000	-0.43952400	3.91606800
H	8.98571700	-2.44689900	3.43815400
C	11.18121800	-2.54770400	3.76697200
C	11.18660200	-0.52746300	4.79284800

H	8.97182000	-0.42506100	4.48965300
C	12.16233400	-1.38196200	3.96860500
C	10.84446600	-1.50521200	5.95040600
C	10.84909700	-2.90214600	5.25213100
H	11.53136800	-3.39736400	3.16774800
H	11.54684100	0.45509000	5.12246200
H	12.48389100	-0.93630300	3.02655700
H	13.04713500	-1.67353500	4.55609400
H	9.88436300	-1.26948500	6.43329500
H	11.62253800	-1.44454400	6.72629600
H	9.89369900	-3.43670200	5.35789100
H	11.63647200	-3.55448800	5.66043500
C	10.16781000	3.23050700	3.43092700
C	10.97210200	4.36997700	3.48108400
C	12.30526900	4.30138200	3.06658300
C	12.81610900	3.08596400	2.59725000
C	12.01296300	1.94525200	2.55060300
H	9.12710500	3.29123900	3.75873500
H	10.55547600	5.31268600	3.84227900
H	12.93861700	5.19051200	3.09715600
H	13.84999500	3.02785900	2.24942100
H	12.40641200	1.02310100	2.12690000

trans- 1D

Energy: -6955.203097

C	0.29576500	-0.70906800	3.34782700
C	0.57652200	1.96220300	3.03861100
Ru	0.01052200	0.47120200	1.73645800
Cl	-2.37122600	0.28530900	2.17774600
Cl	2.38170400	0.44072900	1.04952100
P	-0.36751300	0.09385500	-0.68264100
C	0.83278900	1.00123700	-1.79787100
C	-0.16124500	-1.72954400	-1.08239100
C	-2.14948400	0.46560900	-1.16010700
C	-2.49120500	1.96704200	-1.06077100
C	-4.00652200	2.18982400	-1.18588100
C	-4.55481300	1.59639600	-2.48915500
C	-4.19165200	0.11148600	-2.61262500
C	-2.67386500	-0.11970400	-2.48831000
C	0.96920000	2.50392600	-1.47359500
C	2.14437300	3.11384800	-2.25463500
C	2.00852000	2.88258600	-3.76520600
C	1.82897300	1.39405100	-4.08784200
C	0.64649400	0.78493000	-3.31267100
C	1.29557900	-2.23104900	-1.05547700
C	1.36351200	-3.70838100	-1.47873100
C	0.47257500	-4.59836200	-0.60372600
C	-0.97272100	-4.08608300	-0.59573600
C	-1.05002500	-2.60943400	-0.17744700
H	1.78723700	0.54393300	-1.49332100
H	-0.52849000	-1.82632600	-2.11914500
H	-2.69166900	-0.02277300	-0.33410400
H	-2.13560900	2.37786400	-0.10519400
H	-1.98450400	2.51702500	-1.86970700
H	-4.22476500	3.26877400	-1.13287100
H	-4.50710700	1.72270900	-0.32145900
H	-4.13079200	2.14630500	-3.34947700
H	-5.64870700	1.72519100	-2.54047000
H	-4.54562800	-0.29319500	-3.57524200
H	-4.70897500	-0.45722800	-1.82050400
H	-2.16981900	0.35458500	-3.34393000
H	-2.47119900	-1.19821300	-2.55682200
H	0.04505400	3.03988800	-1.73837700
H	1.13381900	2.63835300	-0.39545100
H	3.08399900	2.66317300	-1.89164800
H	2.20790100	4.19312200	-2.03861200
H	2.88729000	3.28558700	-4.29478000
H	1.13482300	3.44264200	-4.14425200
H	2.75223600	0.84586000	-3.82943800
H	1.67106200	1.25153300	-5.17020400
H	0.55654700	-0.28474100	-3.55650500
H	-0.28314700	1.27036800	-3.64864500
H	1.92934600	-1.62998000	-1.72174900
H	1.71057800	-2.10401700	-0.04496300
H	2.41004600	-4.05095200	-1.43987600
H	1.04789700	-3.80340800	-2.53302400
H	0.86352700	-4.60028900	0.43051400
H	0.50355700	-5.64114400	-0.96432700
H	-1.59657500	-4.69332000	0.07977000
H	-1.40646400	-4.20204700	-1.60493800
H	-0.71139300	-2.50561400	0.86598200
H	-2.09536900	-2.27111400	-0.19189000
H	1.65415100	2.12457000	2.93158600
C	-0.16015500	3.23898500	3.15576400
C	0.27211300	0.77184400	4.00544100
H	-0.65061600	-1.23871300	3.51535700
C	1.50784000	-1.39331100	3.97056500
C	1.43423600	0.59257000	5.04431900

H	-0.70652200	0.92846900	4.47088800
C	2.47841600	-0.24514700	4.29299100
C	0.93654200	-0.40513800	6.12125000
C	1.03972400	-1.78809800	5.40441300
H	1.90363500	-2.22867700	3.37913800
H	1.76684100	1.55956100	5.44473300
H	2.89329100	0.23051900	3.39993100
H	3.29936400	-0.56306000	4.95508900
H	-0.08281700	-0.17340800	6.46289500
H	1.59427200	-0.35701300	7.00224800
H	0.08951400	-2.34200500	5.40338700
H	1.79684000	-2.43061900	5.88003300
C	0.55341700	4.42765700	2.88680500
C	-0.04922900	5.67981800	3.01712100
C	-1.38380700	5.77379100	3.42318800
C	-2.10776600	4.60463800	3.68534700
C	-1.51052900	3.35235300	3.54399000
H	1.60037800	4.36088900	2.58193300
H	0.52777700	6.58380900	2.80918100
H	-1.85981800	6.75079000	3.53025900
H	-3.15456300	4.66645800	3.99090600
H	-2.10237200	2.45109900	3.70287700

A note on structures for 1B and 2B by M06-L/DZQS

The active structures of **1B** and **2B** are transition states. In each case the transition state is between the global minimum inactive structure and a local minimum inactive structure. The energetic and structural relationships of these structures are as follows (where the structures were optimized by M06-L/DZQS, and the energies are from single point calcuations with M06-L/TZQS):

	Global minimum	TS	local minimum
1B			
τ (deg)	168.3	105.3	39.8
Relative energy (kcal/mol)	35.13	48.54	40.46
2B			
τ (deg)	164	100.6	74.7
Relative energy (kcal/mol)	39.40	44.16	42.70

The zero of energy is **1A**(active) for **1B**, and **2A**(active) for **2B**.

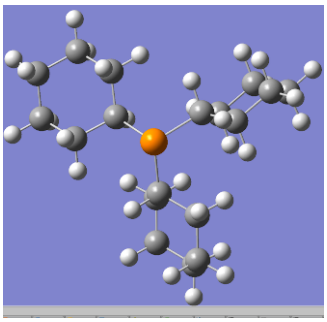
The table shows that it is unambiguous to call the **1B** active carbene a saddle point because the saddle point has τ =105.3 deg, which is reasonably close to the "ideal" value of 90 deg, and the **1B** local minimum has τ = 39.8 deg, which is very far from 90 deg. However, **2B** shows less ideal behavior. The **2B** saddle point has τ =100.6 deg, and the **2B** local minimum has tτ = 74.7deg; both are close to 90 deg with an energy difference of just 1.5 kcal/mol, and either could be considered to be the active carbene of **2B**. In the text we take the active structure as the one with τ closer to 90 deg, that is, the saddle point. However, because the energies of the two structures are so similar, the arguments in the text are not changed if one makes the opposite choice.

One the following pages we give the structures optimized with M06-L/DZQS.

Structures for 1 and 2 by M06-L/DZQS

Cartesian coordinates in angstroms and energies in hartrees

PCy_3



Energy: -1047.29443582

P	-0.23673000	-0.07033800	-1.10347800
C	0.76246800	-1.45952400	-0.34545400
H	0.06419600	-2.30813300	-0.44166900
C	1.97605400	-1.82910800	-1.20840600
H	2.72533800	-1.02696200	-1.16206700
H	1.67672300	-1.90616600	-2.26049400
C	2.61601000	-3.12915800	-0.73018600
H	1.90263000	-3.95464700	-0.87354200
H	3.49298600	-3.37007000	-1.34258900
C	2.99804900	-3.04942200	0.74367900
H	3.43454600	-3.99645200	1.08160500
H	3.78018500	-2.28589600	0.87157700
C	1.79664400	-2.67702300	1.60468400
H	1.04747000	-3.48127100	1.54928400
H	2.08670700	-2.59866600	2.65935800
C	1.16120800	-1.37202100	1.12874400
H	1.88936600	-0.55717800	1.25720700
H	0.29508800	-1.11421000	1.75249500
C	0.52360100	1.54387700	-0.51670800
H	-0.00937100	2.28745800	-1.13476200
C	1.99747200	1.61681500	-0.92875600
H	2.57466500	0.91352000	-0.30967300
H	2.12179100	1.28601800	-1.96814900
C	2.56765900	3.01640200	-0.73556100
H	2.04543500	3.71428100	-1.40654800
H	3.62481300	3.04122900	-1.02511300
C	2.39500400	3.47815200	0.70621000
H	2.77964600	4.49633300	0.83700000
H	2.99790000	2.83361700	1.36367000
C	0.93391900	3.39960000	1.13523500
H	0.82161000	3.71115600	2.18069200
H	0.34451000	4.11078300	0.53681500
C	0.36155700	1.99546500	0.94003600
H	-0.69392700	1.97940300	1.23855900
H	0.87975100	1.29780800	1.61124500
C	-1.80034200	-0.12499300	-0.07654200
H	-1.55864800	0.01638900	0.99062200
C	-2.51941800	-1.47001000	-0.21971300
H	-1.88663800	-2.28560200	0.15061300
H	-2.68948300	-1.67272900	-1.28876600
C	-3.85315800	-1.48670000	0.52008500
H	-4.34966800	-2.45385200	0.37757100
H	-3.66621200	-1.39244400	1.60024100

C	-4.75714500	-0.34624000	0.06988800
H	-5.01815100	-0.48883700	-0.98932100
H	-5.70202000	-0.36012100	0.62538700
C	-4.05596200	0.99602600	0.23458000
H	-3.87258700	1.18030300	1.30410900
H	-4.69797700	1.81414700	-0.11285600
C	-2.72729000	1.01730300	-0.51326800
H	-2.91546900	0.92153900	-1.59372800
H	-2.23223500	1.98767200	-0.37787000

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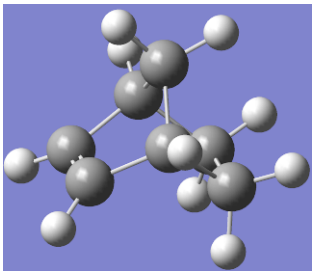
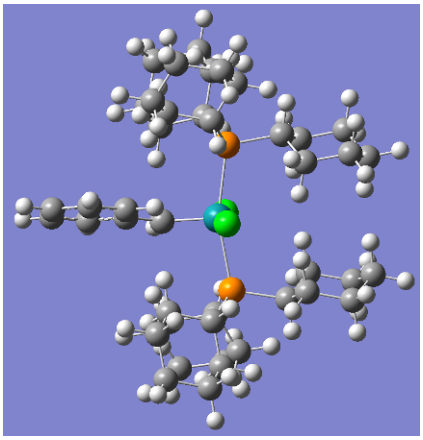


Energy: -272.769373094

C	-1.27219000	0.67050700	-0.49837600
C	-1.27184900	-0.67088100	-0.49862800
C	-0.08537500	-1.12077600	0.32324500
C	-0.08572600	1.12063500	0.32362600
C	1.17703700	-0.77340900	-0.51870300
C	1.17651400	0.77404600	-0.51872300
C	-0.03235600	-0.00022400	1.37108000
H	-1.90922700	-1.32726600	-1.08295700
H	-1.90979500	1.32710000	-1.08223100
H	-0.11071800	-2.14946600	0.69078800
H	-0.11169400	2.14916800	0.69157700
H	2.07673500	-1.17050100	-0.03587200
H	1.12845400	-1.20271800	-1.52341900
H	2.07634200	1.17181500	-0.03670400
H	1.12698100	1.20315800	-1.52349100
H	0.89330800	-0.00022100	1.95965300
H	-0.89671100	-0.00045300	2.04152800

1Aa



Energy: -3379.58022925

Ru	-0.02951500	0.01748500	0.06771700
Cl	-0.08202100	-0.28563300	-2.38715100
Cl	-0.02930500	0.83989300	2.41726900
P	-2.44677900	0.26627200	-0.02922500
C	-0.00642400	-1.71529600	0.76926800
H	-0.24444900	-1.73150300	1.84798900
C	-3.31058600	-0.76053900	-1.30373300
H	-2.89981900	-0.34988800	-2.23919700
C	-2.89767200	-2.23422100	-1.29218900
H	-3.23220100	-2.72292900	-0.36641000
H	-1.80660300	-2.29882500	-1.31202900
C	-3.49185600	-2.96220300	-2.49299000
H	-3.04984400	-2.54595900	-3.41045200
H	-3.20781500	-4.02092100	-2.46646100
C	-5.00873800	-2.81227700	-2.54616300
H	-5.41701700	-3.32026900	-3.42764700
H	-5.45212100	-3.31015900	-1.67017100
C	-5.41818000	-1.34365700	-2.54130900
H	-5.05518700	-0.86230200	-3.46167300
H	-6.51018500	-1.24564900	-2.54997300
C	-4.83369300	-0.61127800	-1.33629100
H	-5.26113700	-1.03682000	-0.41591200
H	-5.12659900	0.44704800	-1.35373800
C	-3.27173000	0.06314300	1.62441100
H	-2.52195300	0.50989500	2.29534800
C	-3.39995500	-1.40991300	2.02499200
H	-4.17499900	-1.89191100	1.40950700
H	-2.46467800	-1.94819400	1.82394800
C	-3.78644300	-1.53046200	3.49474400
H	-2.98066200	-1.10333900	4.10902800
H	-3.87235800	-2.58584800	3.77916100
C	-5.09033800	-0.79240500	3.77403400
H	-5.35218300	-0.85844400	4.83632500
H	-5.90639400	-1.28438700	3.22314000
C	-5.00062200	0.66524200	3.33823700
H	-5.95347900	1.17954500	3.51086600
H	-4.25111000	1.18065900	3.95626500
C	-4.59627100	0.79556200	1.87031500
H	-4.51266000	1.85801800	1.61392000
H	-5.39092000	0.38130600	1.23350700
C	-2.86358600	2.01104100	-0.51291800
H	-3.94686400	2.12488800	-0.34387000
C	-2.59449900	2.33730700	-1.98400700
H	-3.14240500	1.65195800	-2.64106100
H	-1.52958200	2.18085000	-2.21068100

C	-2.99223700	3.77666400	-2.29579100
H	-2.78597500	4.00065300	-3.34865300
H	-4.07929600	3.88758500	-2.16332900
C	-2.27075500	4.76252300	-1.38670200
H	-1.19121500	4.70675500	-1.59379000
H	-2.57431800	5.79174800	-1.61054800
C	-2.51368300	4.43836100	0.08304400
H	-3.57875700	4.58842700	0.31782600
H	-1.95652700	5.12729900	0.72949200
C	-2.12992300	2.99902600	0.40337600
H	-1.04235900	2.87049300	0.26995900
H	-2.30764300	2.76707300	1.46134000
C	0.80384300	-5.69530800	-0.52587800
C	0.47974800	-5.41865800	0.80192500
C	0.21670600	-4.11032200	1.18870900
C	0.27577300	-3.04689200	0.26187900
C	0.60321000	-3.34860500	-1.07643500
C	0.86172200	-4.65696500	-1.45951600
H	1.01160300	-6.71675000	-0.83369200
H	0.43177400	-6.22137700	1.53264100
H	-0.03583500	-3.88496000	2.22369400
H	0.64260700	-2.53783000	-1.80078200
H	1.11410600	-4.87256300	-2.49460800
P	2.35307200	0.49729000	0.03183700
C	3.24983300	0.21923600	1.62878800
H	2.72566900	0.92555500	2.29136900
C	4.73615100	0.58942500	1.60768000
H	4.88483000	1.58519700	1.16865600
H	5.28490600	-0.11704000	0.96662700
C	5.31588000	0.53865300	3.01954300
H	6.38297900	0.78953200	2.99879800
H	4.82632200	1.31073200	3.63174000
C	5.09405900	-0.82593000	3.66106800
H	5.49815500	-0.83887400	4.67993800
H	5.65649700	-1.58437100	3.09548400
C	3.61521000	-1.19723500	3.66408300
H	3.46735200	-2.18934900	4.10611300
H	3.06119200	-0.48850900	4.29673900
C	3.02712000	-1.15781800	2.25765000
H	1.95269900	-1.36609000	2.29563000
H	3.48870600	-1.94509500	1.64640500
C	2.53849800	2.32550100	-0.26273800
H	3.58837500	2.49576300	-0.55164800
C	2.25317700	3.20104100	0.96011300
H	2.91442700	2.93485800	1.79342700
H	1.22990400	3.01566200	1.31767200
C	2.43160800	4.67664300	0.61503200
H	2.22112700	5.29260900	1.49666000
H	3.48380700	4.86409500	0.35094600
C	1.53963300	5.08659000	-0.54929300
H	0.48826900	4.97576600	-0.24247200
H	1.67945000	6.14604300	-0.79383600
C	1.79690400	4.21459300	-1.77251700
H	2.81817600	4.39514800	-2.14154300
H	1.12136800	4.48471400	-2.59386700
C	1.64178300	2.73676500	-1.43757300
H	1.82476900	2.10583400	-2.31679400
H	0.58894400	2.54213900	-1.16330900
C	3.27860200	-0.28124200	-1.38095700
H	2.50269600	-0.32782800	-2.16273300
C	4.47478900	0.47508300	-1.96898000
H	5.27443200	0.56785500	-1.21901300
H	4.19264400	1.49566700	-2.25259500
C	5.00881200	-0.25486100	-3.20113700
H	4.23576900	-0.23330800	-3.98287500
H	5.87478200	0.28144000	-3.60677800
C	5.36752200	-1.70441900	-2.89688100
H	5.72151500	-2.20894100	-3.80329000
H	6.20392400	-1.72788000	-2.18201000

C	4.17944700	-2.44514500	-2.29485800
H	4.44674500	-3.47999700	-2.05039800
H	3.36564100	-2.49815400	-3.03379200
C	3.67213400	-1.72480500	-1.05137600
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H	4.46959400	-1.71994100	-0.29330500

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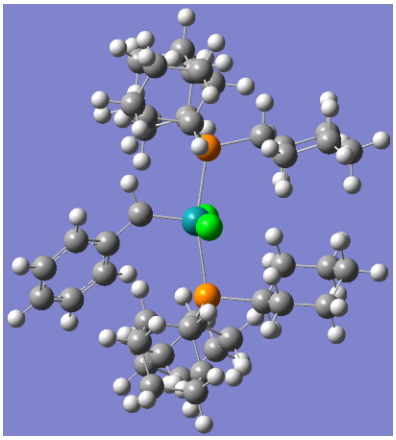

Energy: -3379.56411586

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P	-2.29506200	0.52606200	-0.01546500
C	0.13041500	-1.98168700	0.04123400
H	1.09425100	-2.46469600	-0.16501200
C	-3.26355500	0.09499700	-1.54334600
H	-2.64957500	0.61613200	-2.29532300
C	-3.21264300	-1.37578200	-1.95713200
H	-3.77565800	-2.00405400	-1.25083400
H	-2.17376100	-1.71848100	-1.93219400
C	-3.78157200	-1.54851500	-3.36274100
H	-3.11498400	-1.03804600	-4.07359500
H	-3.77416700	-2.60984900	-3.63921400
C	-5.18654700	-0.97021100	-3.48774100
H	-5.55744300	-1.07937600	-4.51357500
H	-5.87293200	-1.54548700	-2.84804700
C	-5.22102500	0.49338800	-3.05885400
H	-4.60221600	1.08942000	-3.74647800
H	-6.23936100	0.89396300	-3.12933300
C	-4.68675300	0.65056100	-1.63779900
H	-5.34503100	0.09695600	-0.95824200
H	-4.72717400	1.70035100	-1.31883200
C	-3.28711400	0.23887200	1.56277400
H	-2.53064600	-0.24325400	2.20062100
C	-4.47248300	-0.72471000	1.43404900
H	-5.31287900	-0.20242900	0.95869100
H	-4.23510100	-1.57901000	0.79302400
C	-4.92092600	-1.19174000	2.81452000
H	-4.09217600	-1.72520300	3.30513800
H	-5.74562400	-1.90975000	2.72532100
C	-5.33733400	-0.00093000	3.67013600
H	-5.61686500	-0.32523800	4.67918100
H	-6.23852000	0.45253500	3.23090700
C	-4.23127400	1.04661600	3.73718900
H	-4.56922200	1.92407500	4.30077600
H	-3.37275600	0.63632700	4.28844700
C	-3.74813500	1.47146300	2.35079900
H	-2.93896900	2.20071000	2.46130500
H	-4.56318200	1.97742100	1.80983500
C	-2.21178500	2.40676400	-0.15014800
H	-3.13341900	2.80312700	0.30321200
C	-2.11540100	2.97460000	-1.57149500
H	-2.97888800	2.67982200	-2.17654700

H	-1.22850000	2.55902200	-2.06853700
C	-2.02453000	4.49917000	-1.54713000
H	-1.95807000	4.87879300	-2.57329500
H	-2.95337100	4.91251800	-1.12473700
C	-0.84114000	4.98193300	-0.71949100
H	0.09122500	4.63871000	-1.19482900
H	-0.79573100	6.07722000	-0.70332600
C	-0.91510300	4.41964300	0.69287300
H	-1.80134800	4.82585000	1.20416300
H	-0.04852000	4.72905900	1.29127500
C	-1.01602100	2.90149300	0.67158100
H	-0.09734500	2.49338100	0.20564700
H	-1.02430100	2.49506300	1.68785000
C	-2.96164100	-4.90280300	-0.02546000
C	-2.98120900	-3.90648000	0.94959000
C	-1.99462200	-2.92576700	0.96943500
C	-0.94724800	-2.95173500	0.03602000
C	-0.90791900	-3.99662800	-0.90971100
C	-1.92402800	-4.94077800	-0.96012800
H	-3.74423900	-5.65619100	-0.05064400
H	-3.77434600	-3.88856400	1.69366800
H	-1.98964700	-2.14656200	1.72868800
H	-0.08692500	-4.03084800	-1.62381900
H	-1.90096400	-5.72050900	-1.71684000
P	2.54830200	-0.04156100	0.04985900
C	3.35145700	-0.78914400	1.55417200
H	3.00041700	-0.10623800	2.34377400
C	4.88246900	-0.79000300	1.56542900
H	5.28326000	0.19266200	1.28559500
H	5.24906100	-1.50157400	0.81010300
C	5.41657400	-1.20591400	2.93290100
H	6.51300200	-1.20420300	2.92682700
H	5.10820900	-0.45892800	3.67939500
C	4.87998700	-2.57341700	3.33661800
H	5.24920000	-2.85391400	4.32994200
H	5.26715100	-3.33039100	2.63774300
C	3.35675400	-2.59162400	3.30554900
H	2.97608800	-3.58504400	3.56929000
H	2.96838900	-1.89985300	4.06732800
C	2.80687100	-2.16637500	1.94758400
H	1.71372400	-2.12469200	1.99310200
H	3.07873700	-2.91546300	1.18789200
C	3.13580000	1.72457800	0.12894800
H	4.23667700	1.67236000	0.10199400
C	2.75468200	2.45973600	1.41740000
H	3.08552900	1.90462100	2.30277000
H	1.66073800	2.51951000	1.50302200
C	3.36194700	3.86055000	1.43314300
H	3.06560600	4.38517400	2.34926000
H	4.45854800	3.77238700	1.46947300
C	2.96699600	4.66917900	0.20320500
H	1.88465500	4.86162400	0.22981400
H	3.45282300	5.65188500	0.21760400
C	3.30090600	3.92444300	-1.08303100
H	4.39367900	3.82969700	-1.17927000
H	2.96317600	4.49389200	-1.95718500
C	2.67861700	2.53227700	-1.09277400
H	2.91092100	2.01125200	-2.02938000
H	1.58158400	2.61497900	-1.08122200
C	3.40383000	-0.66224000	-1.49158900
H	2.72130500	-0.30452100	-2.27882200
C	4.80324700	-0.11135500	-1.81250900
H	5.52953000	-0.46051900	-1.06614100
H	4.82188400	0.98272200	-1.77251900
C	5.24930500	-0.57355600	-3.19810600
H	4.56230700	-0.15709400	-3.94945700
H	6.24129400	-0.16600600	-3.42576500
C	5.25410300	-2.09284000	-3.30766100
H	5.55584800	-2.40689000	-4.31350900

H	6.00690200	-2.50140400	-2.61660200
C	3.88746200	-2.66386400	-2.95393500
H	3.90444600	-3.75950600	-2.98917400
H	3.15048500	-2.33871100	-3.70244300
C	3.42442600	-2.19294700	-1.58002700
H	2.43180100	-2.60632500	-1.37593300
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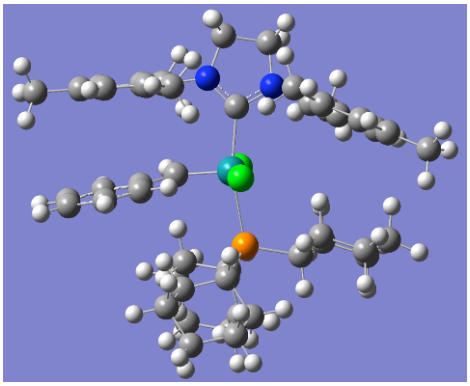
2Aa



Energy: -3257.83455408

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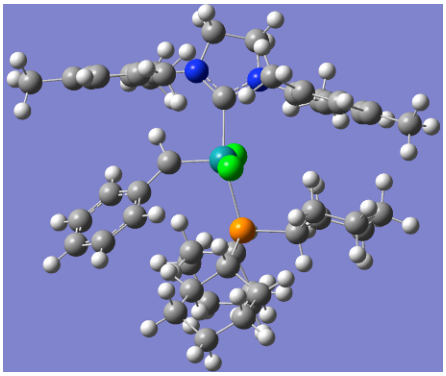
C	-1.75377900	0.33435500	0.34291600
H	-2.07867200	0.29332600	1.39796600
C	-4.78306800	2.30352900	-1.92049700
C	-4.84370900	2.24169500	-0.52876500
C	-3.84465800	1.58264900	0.17703600
C	-2.74958500	0.98984500	-0.48803900
C	-2.70112700	1.07168300	-1.89398500
C	-3.71156100	1.71338800	-2.59638300
C	-0.58875600	-2.41763200	0.23087400
N	-1.79403900	-2.95110500	0.55011800
C	-1.75112700	-4.42014500	0.65127900
C	-0.25993800	-4.69949500	0.71167100
N	0.30745500	-3.43055700	0.23710400
C	4.39050200	-3.33463400	-0.83075300
C	4.00578100	-3.22467400	0.50527900
C	2.66352600	-3.23167700	0.89757300
C	1.69051500	-3.34294700	-0.10746500
C	2.04099200	-3.52099700	-1.45980600
C	3.39256500	-3.49001100	-1.79833600
C	-5.64335800	-1.26217300	0.20835400
C	-4.91709600	-1.61698400	-0.93185700
C	-3.63256800	-2.15233500	-0.84869300
C	-3.07261500	-2.32893100	0.42847300
C	-3.76998800	-1.98944100	1.59579000
C	-5.05314000	-1.45277000	1.45934400
C	2.30203900	-3.19867400	2.34921300
C	0.99050800	-3.79025000	-2.48956600
C	5.83616300	-3.29079400	-1.22184200
C	-2.84305300	-2.47333200	-2.07663000
C	-3.13371600	-2.16295600	2.93791600
C	-7.01629700	-0.67698700	0.08136800
H	-5.56539800	2.81308200	-2.47743400
H	-5.67260000	2.70071500	0.00437000
H	-3.89381000	1.51504300	1.26270000
H	-1.85370800	0.63232500	-2.41424900
H	-3.65977300	1.76654700	-3.68104100
H	-2.29628300	-4.75924500	1.53759400
H	-2.23262200	-4.86590400	-0.23225400
H	0.08980000	-4.90556700	1.73298300
H	0.05783500	-5.52719400	0.06920300
H	4.77187500	-3.13483700	1.27532600
H	3.67391900	-3.61297800	-2.84347000
H	-5.35542800	-1.45643900	-1.91651500

H	-5.60296300	-1.17206700	2.35712200
H	1.32367400	-2.74501300	2.52379100
H	2.29338700	-4.21388300	2.76707700
H	3.03514400	-2.62581200	2.92443500
H	1.44215900	-4.00271300	-3.46133900
H	0.36967000	-4.65036600	-2.20879200
H	0.32385000	-2.92997600	-2.60685100
H	6.07828900	-4.05891400	-1.96260400
H	6.09651700	-2.32446600	-1.67128800
H	6.49185800	-3.43071000	-0.35804100
H	-1.96276600	-1.82083100	-2.16275600
H	-2.46097500	-3.50141200	-2.06713300
H	-3.44718500	-2.34521100	-2.97809500
H	-3.79500800	-1.81513400	3.73528000
H	-2.88976000	-3.21241900	3.14233200
H	-2.18646800	-1.61125600	2.99923200
H	-7.44773900	-0.44440800	1.05850400
H	-6.99717900	0.24820500	-0.50636700
H	-7.70037000	-1.36120900	-0.43205000
P	1.16156500	1.75175900	0.16099700
C	0.93656100	2.82847200	-1.34251500
C	-0.34513600	3.66579900	-1.26337200
C	-0.65790900	4.30177500	-2.61282200
C	0.49973100	5.17716900	-3.07684700
C	1.80146300	4.38536800	-3.11329500
C	2.10871500	3.71952600	-1.77226700
C	0.91601000	2.76311200	1.69557900
C	-0.54493700	3.02495100	2.07312600
C	-0.62937900	3.64971500	3.46234500
C	0.19256500	4.93078600	3.55039600
C	1.64149100	4.68140000	3.14981700
C	1.73550600	4.05652400	1.75987300
C	2.98988500	1.42922600	0.17494900
C	3.41221200	0.54746400	-1.00511200
C	4.93250400	0.50180600	-1.10388900
C	5.56374300	0.00928000	0.19437000
C	5.06430000	0.78649100	1.40760400
C	3.53895900	0.83467000	1.47353800
H	0.78722700	2.07778500	-2.13529400
H	-1.18967100	3.05865200	-0.92061400
H	-0.21241500	4.46406300	-0.51690000
H	-0.83702900	3.50421800	-3.34918900
H	-1.58718000	4.88097600	-2.55144700
H	0.28928300	5.61315100	-4.06043700
H	0.61111300	6.02197300	-2.38043100
H	1.72578500	3.60303900	-3.88251500
H	2.63719400	5.03026200	-3.40988100
H	2.29781300	4.49060000	-1.01047900
H	3.03393800	3.14103400	-1.86731800
H	1.29351600	2.07654200	2.46885100
H	-1.02018200	3.69478100	1.34409400
H	-1.09797800	2.08047000	2.05664400
H	-1.67623500	3.84554000	3.72272000
H	-0.25714500	2.92150500	4.19752600
H	-0.24027000	5.68531600	2.87588400
H	0.14189800	5.35511500	4.55993300
H	2.21916900	5.61281000	3.18403100
H	2.10751000	3.99948200	3.87673200
H	2.78713900	3.87566800	1.50222600
H	1.35241800	4.77106700	1.01581400
H	3.46527000	2.41514300	0.04649000
H	3.01336200	-0.46919100	-0.85272800
H	2.96844700	0.88825800	-1.94843200
H	5.23643300	-0.13466900	-1.94482700
H	5.30457700	1.51234800	-1.33500300
H	5.30480700	-1.04812800	0.32822900
H	6.65804100	0.05636100	0.13238600
H	5.46802600	0.35133000	2.32986500
H	5.44360100	1.81934200	1.36343600

H	3.22752100	1.41836200	2.34722500
H	3.12029100	-0.17307200	1.61847900

2Ai



Energy: -3257.80783455

Ru	-0.28463500	-0.36719400	-0.10902400
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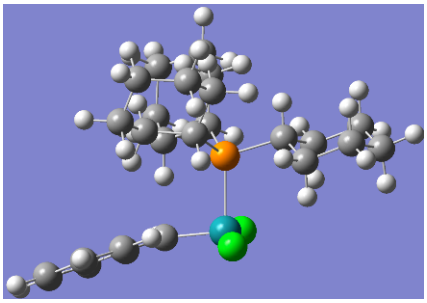
Cl	-0.20473400	-0.50056100	2.34208100
C	-1.81395900	0.67484900	-0.25354600
H	-2.66610000	0.17077400	0.20975800
C	-3.00656700	4.70243600	-0.87884300
C	-3.39282300	4.01559800	0.27617900
C	-2.99621200	2.69997700	0.46686800
C	-2.13550000	2.07305000	-0.45709300
C	-1.74401900	2.77736100	-1.60780600
C	-2.20168000	4.07344000	-1.82722900
C	-1.40093800	-2.16899900	0.16179100
N	-2.70084300	-2.42956300	0.46108100
C	-2.93929200	-3.84688800	0.78585700
C	-1.53719700	-4.36101200	1.03703500
N	-0.71719400	-3.31647200	0.40623800
C	3.18590600	-4.43802600	-0.75147600
C	2.87447300	-4.22879000	0.59112700
C	1.60611000	-3.81604800	1.00853000
C	0.62673400	-3.60477300	0.02472600
C	0.88593400	-3.87064600	-1.33618400
C	2.17546600	-4.25415300	-1.70012800
C	-6.09408500	-0.05154400	-0.34282200
C	-5.35804200	-0.61653100	-1.38845900
C	-4.23334400	-1.40904800	-1.15778000
C	-3.84846100	-1.63084900	0.17522500
C	-4.56481700	-1.08756000	1.25206700
C	-5.68667000	-0.30549200	0.96784600
C	1.30855500	-3.67583700	2.46834000
C	-0.21403300	-3.83297900	-2.34822600
C	4.56210800	-4.85857100	-1.16787400
C	-3.41623500	-1.93542900	-2.29451200
C	-4.07408300	-1.26138100	2.65539100
C	-7.26995300	0.83136200	-0.62914300
H	-3.34457700	5.72230500	-1.04227800
H	-4.02622200	4.50242600	1.01331700
H	-3.32664400	2.13979100	1.34101400
H	-1.09738300	2.27518000	-2.32778600
H	-1.91424800	4.60291300	-2.73225000
H	-3.60154900	-3.93911800	1.65160100
H	-3.42924000	-4.33781500	-0.06873100
H	-1.30162600	-4.42685100	2.10809000
H	-1.33653800	-5.33449400	0.57868500
H	3.64178100	-4.39034000	1.34806800
H	2.38541700	-4.44908500	-2.75102400
H	-5.65835600	-0.42302600	-2.41766000

H	-6.23909600	0.14031100	1.79428000
H	0.56185300	-2.90104800	2.65923200
H	0.93690600	-4.62113700	2.88497100
H	2.21342600	-3.41906400	3.02721500
H	0.14128000	-4.18424300	-3.31963000
H	-1.05064800	-4.47305900	-2.03943600
H	-0.60618100	-2.82092700	-2.48339700
H	4.53391900	-5.72654800	-1.83414200
H	5.07570700	-4.05844700	-1.71409900
H	5.18290900	-5.11452300	-0.30509400
H	-2.47349900	-1.37847900	-2.39488700
H	-3.13910400	-2.98537200	-2.15035900
H	-3.95699100	-1.85125600	-3.24006800
H	-4.65379800	-0.65050800	3.35163500
H	-4.14479500	-2.30128400	2.99647700
H	-3.01623900	-0.98042900	2.73912800
H	-7.82251600	1.07516800	0.28173300
H	-6.95173400	1.77620800	-1.08459900
H	-7.96676300	0.36259800	-1.33126200
P	1.51936000	1.34904300	0.08550000
C	1.83177400	2.56083500	-1.31901300
C	1.19782800	3.93450700	-1.06944600
C	1.20647000	4.77446400	-2.34031100
C	2.62870200	4.97592700	-2.84643300
C	3.32953800	3.63644600	-3.03215700
C	3.28351200	2.77754600	-1.76934800
C	1.57391600	2.26924200	1.70154600
C	0.29566600	3.03873800	2.04511900
C	0.33059100	3.50161900	3.49754000
C	1.57077800	4.34195400	3.78078600
C	2.84314700	3.57965200	3.42740100
C	2.82772900	3.10662900	1.97506600
C	3.13573300	0.41798000	0.17109500
C	3.32174400	-0.56524400	-0.98977700
C	4.77976500	-1.00747100	-1.05029300
C	5.24328800	-1.62624500	0.26454700
C	4.89671500	-0.76584600	1.47592900
C	3.43535000	-0.31776700	1.48030900
H	1.29675900	2.08606100	-2.15825300
H	0.18176300	3.83840300	-0.68622300
H	1.76900700	4.46299600	-0.29339700
H	0.61198500	4.26140400	-3.11239600
H	0.71524800	5.73872500	-2.15951800
H	2.63430100	5.54582700	-3.78294400
H	3.18651600	5.57799900	-2.11360800
H	2.84028400	3.08279100	-3.84664800
H	4.37054600	3.78550700	-3.34286900
H	3.84760500	3.27287400	-0.96278200
H	3.79103500	1.82907800	-1.96878100
H	1.58460000	1.42361500	2.40553300
H	0.17867000	3.91516900	1.39437600
H	-0.57114400	2.39147800	1.87285800
H	-0.57971200	4.06561700	3.73460000
H	0.32874800	2.61692800	4.15104900
H	1.52719100	5.26349600	3.18026800
H	1.59358900	4.65855000	4.83010400
H	3.72986400	4.19710400	3.61491200
H	2.93125200	2.70146800	4.08470600
H	3.73917700	2.53346400	1.76197900
H	2.85520800	3.98206400	1.31051700
H	3.90673900	1.19770500	0.07028500
H	2.66133400	-1.43482400	-0.83239500
H	3.00010200	-0.13930700	-1.94664300
H	4.92829100	-1.71464000	-1.87647300
H	5.40114000	-0.12881600	-1.28543400
H	4.75430600	-2.59941600	0.38118400
H	6.32195400	-1.82528700	0.23527100
H	5.12774200	-1.31012300	2.40046300
H	5.53180700	0.13381200	1.48452700

H	3.25318100	0.31044300	2.35887600
H	2.76037000	-1.18134400	1.57891400

1Ba TS

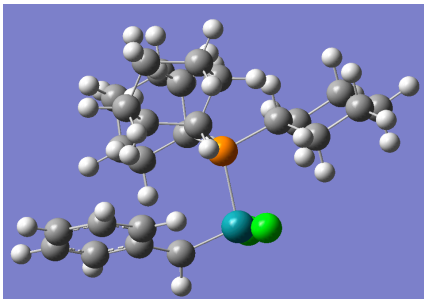


Energy: -2332.204815

Ru	-0.23678300	-1.40527700	-1.19617900
C	-1.80017400	-0.39355200	-1.43053400
C	-5.77232600	-0.29573400	0.08356800
C	-5.36560700	0.57059400	-0.93189400
C	-4.06876500	0.49658200	-1.41924900
C	-3.14765500	-0.44788100	-0.90696300
C	-3.58219000	-1.31912100	0.11501900
C	-4.87805300	-1.23643000	0.60142100
P	0.79884800	0.17310500	0.10263100
C	1.10839500	1.85519200	-0.61295700
C	1.83149000	2.79105600	0.36575500
C	2.23624500	4.09113600	-0.32290600
C	1.02847700	4.78496700	-0.93816900
C	0.31375100	3.85693700	-1.91106800
C	-0.09923000	2.54340200	-1.25302300
C	2.51504100	-0.44685600	0.46158200
C	3.47761400	-0.34459400	-0.72625400
C	4.87394400	-0.81755200	-0.32732000
C	4.85971700	-2.22567400	0.25393200
C	3.88647600	-2.32379100	1.42174200
C	2.49100600	-1.87846400	1.00493000
C	-0.02786000	0.29949100	1.76463100
C	0.86398200	0.59148400	2.97929600
C	0.04870900	0.46029200	4.26548300
C	-1.17640800	1.36504300	4.25936800
C	-2.04212200	1.10675700	3.03168400
C	-1.22684600	1.25344200	1.75152200
H	-1.70010200	0.40620500	-2.18199600
H	-6.78605700	-0.23881900	0.47132300
H	-6.05902000	1.30168300	-1.33737500
H	-3.73805800	1.17559700	-2.20299700
H	-2.87971800	-2.04449000	0.51605300
H	-5.19857100	-1.90952500	1.39191000
H	1.78891200	1.61925700	-1.44509300
H	2.71473200	2.30489100	0.79900700
H	1.16308500	3.02642600	1.20684000
H	2.74353900	4.74903600	0.39210200
H	2.96805600	3.86492500	-1.11235100
H	1.33121600	5.71106400	-1.43960400
H	0.33482700	5.07945000	-0.13585900
H	-0.56693300	4.34761400	-2.34077700
H	0.98205500	3.62995800	-2.75440600
H	-0.51859500	1.88204400	-2.01377400
H	-0.88390600	2.73167000	-0.50747700
H	2.89394700	0.21302300	1.25963600
H	3.53573400	0.68466900	-1.09840300
H	3.09226400	-0.94402900	-1.56359500
H	5.54211700	-0.76250800	-1.19394900
H	5.28443100	-0.12352700	0.42203300

H	4.55459500	-2.93711500	-0.52683800
H	5.86837800	-2.52104200	0.56410200
H	4.23875200	-1.68719300	2.24830300
H	3.85001400	-3.34627400	1.81314400
H	1.77708900	-1.98157800	1.83104300
H	2.11319400	-2.55340300	0.22226800
H	-0.42366200	-0.72169700	1.88368100
H	1.28109000	1.60649700	2.90937200
H	1.71625800	-0.09579600	3.02102100
H	-0.27327700	-0.58588100	4.37002100
H	0.68415400	0.67671200	5.13176500
H	-1.75735000	1.22610000	5.17807600
H	-0.85052400	2.41605400	4.25620900
H	-2.90360700	1.78432000	3.00950500
H	-2.45045200	0.08646900	3.07517500
H	-1.85957200	1.07320700	0.87493700
H	-0.86661100	2.29042900	1.67038000
Cl	-0.70983100	-3.00570700	0.55523900
Cl	0.68675000	-0.41895000	-3.20515500

1B local minimum



Energy: -2332.217698

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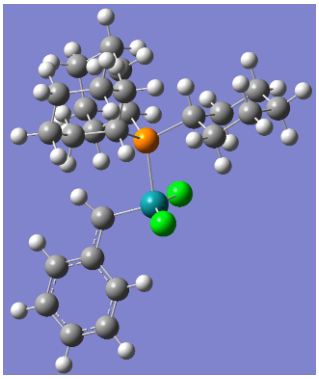
C	-5.27306700	-0.31696300	0.23045100
C	-4.98773600	-0.06368200	-1.11342000
C	-3.78934200	-0.49799000	-1.66397700
C	-2.82628300	-1.14035900	-0.86043100
C	-3.11903700	-1.37798400	0.49477700
C	-4.34567100	-0.99147800	1.02305600
P	0.60434200	0.19466400	0.13023300
C	0.51365900	1.69592000	-0.94921000
C	0.95614300	3.00086100	-0.27560500
C	1.12094000	4.10043200	-1.32195100
C	-0.15614500	4.29065300	-2.13245800
C	-0.59966600	2.98331800	-2.78001100
C	-0.78156700	1.87830800	-1.74392800
C	2.40362100	0.18297000	0.64011900
C	3.41381400	0.47781400	-0.47374600
C	4.82847600	0.52961400	0.09973000
C	5.19429900	-0.75589400	0.83016100
C	4.17375100	-1.07554300	1.91582700
C	2.76455400	-1.13255200	1.33947000
C	-0.33679400	0.48217600	1.72241100
C	0.47528100	1.08065800	2.88107900
C	-0.36482600	1.14058900	4.15459100
C	-1.66073500	1.91453900	3.95264100
C	-2.45192500	1.33688400	2.78711700
C	-1.61181500	1.31352200	1.51593200
H	-1.71099600	-2.14439600	-2.42214900
H	-6.22107900	0.00385800	0.65357700
H	-5.71137800	0.45674200	-1.73497400
H	-3.57472400	-0.32752600	-2.71699000
H	-2.37717400	-1.89270700	1.10325500
H	-4.57448600	-1.20546100	2.06374500
H	1.27531200	1.43564600	-1.69949400
H	1.89608800	2.86147300	0.27428600
H	0.21037200	3.31824900	0.46594600
H	1.41790000	5.03820000	-0.83817800
H	1.94322800	3.82513400	-1.99882000
H	-0.01341900	5.06719800	-2.89230000
H	-0.95389300	4.65316100	-1.46655300
H	-1.52980400	3.12840700	-3.34136900
H	0.15661600	2.66033800	-3.51008100
H	-1.04052300	0.93330200	-2.23549300
H	-1.61660400	2.13549000	-1.07846100
H	2.48980500	0.99801400	1.37586300
H	3.19194600	1.42819800	-0.97200900
H	3.34871500	-0.29557100	-1.24951400
H	5.54397300	0.73304500	-0.70487000
H	4.90197100	1.37680500	0.79907900

H	5.22029000	-1.58506800	0.10887300
H	6.20172900	-0.68310100	1.25521100
H	4.21291400	-0.29874800	2.69515500
H	4.41423300	-2.02297800	2.41071900
H	2.02890600	-1.39128700	2.10987300
H	2.70536800	-1.95273100	0.60655500
H	-0.63670900	-0.53609800	2.01782400
H	0.81106600	2.09429100	2.61011400
H	1.37710100	0.49234900	3.07819800
H	-0.60260400	0.11297100	4.46493900
H	0.22746200	1.57867500	4.96607900
H	-2.25849100	1.90711300	4.87097500
H	-1.42657400	2.96910800	3.74398900
H	-3.37432700	1.90426800	2.61524400
H	-2.76064600	0.30938300	3.02977100
H	-2.19940400	0.93521000	0.67570100
H	-1.33509600	2.34508300	1.25923400
Cl	-0.04243300	-3.13126900	0.97462500
Cl	1.32452600	-1.00882800	-2.90843400

1Bi



Energy: -2332.226187

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Cl	-1.02949200	-2.02046200	1.96905300
Cl	-0.92522900	-1.17228500	-2.53354600
P	0.92224500	0.04588200	-0.00824900
C	-2.18036700	0.44983300	0.10803600
H	-1.83905100	1.49157200	0.15389900
C	1.23407600	1.29824400	-1.34402700
H	1.31473400	0.64725000	-2.22822400
C	2.54574300	2.07634200	-1.19371100
H	3.38596600	1.39829100	-0.99628600
H	2.47512700	2.74725700	-0.32442300
C	2.82430900	2.91068500	-2.44141700
H	3.75964200	3.46839900	-2.31656000
H	2.97671800	2.23501300	-3.29598100
C	1.66693800	3.85388800	-2.74284600
H	1.86946500	4.43030400	-3.65247300
H	1.57725600	4.58655400	-1.92660500
C	0.35896800	3.08493000	-2.87611700
H	-0.47490200	3.76944500	-3.06823800
H	0.41549800	2.41595700	-3.74719100
C	0.06419300	2.24100000	-1.63985700
H	-0.84282500	1.65157000	-1.80687200
H	-0.12156600	2.90059300	-0.77831500
C	2.32868500	-1.15432000	-0.22122900
H	3.23016600	-0.56278900	0.00807400
C	2.50298500	-1.71404900	-1.63544800
H	2.57767400	-0.90974600	-2.37582400
H	1.61587400	-2.29783000	-1.91481800
C	3.75265900	-2.58768000	-1.70698300
H	3.86373400	-2.99336200	-2.71873500
H	4.63906000	-1.96047000	-1.52672500
C	3.71956200	-3.71233500	-0.67852200
H	2.89757200	-4.39985600	-0.92366000
H	4.64161600	-4.30268100	-0.72566500
C	3.50393300	-3.16385200	0.72686200
H	4.37403400	-2.55669800	1.02121600
H	3.43602900	-3.97926100	1.45542800
C	2.24793900	-2.30363700	0.79105500
H	2.07646200	-1.93045400	1.80819200
H	1.36769900	-2.92048600	0.56142500
C	1.23875400	0.76871700	1.68183800
H	0.78522500	0.00834800	2.33754500
C	2.70897400	0.92328100	2.09829700
H	3.21746000	1.64228600	1.44186700
H	3.24622400	-0.02559900	1.99813200
C	2.80956700	1.40144400	3.54484400
H	2.39302300	0.62605700	4.20399900

H	3.86356500	1.51210900	3.82455500
C	2.05256100	2.70416400	3.76378200
H	2.12556200	3.02034800	4.81034200
H	2.52032100	3.50106800	3.16597900
C	0.59510100	2.55356400	3.35023400
H	0.05417700	3.49804800	3.47842900
H	0.10368200	1.82117300	4.00605100
C	0.47558100	2.07894300	1.90552700
H	-0.57934900	1.94792500	1.64244500
H	0.87654000	2.85612700	1.23657000
C	-6.40461300	-0.04124900	0.11388500
C	-5.84035200	1.21865800	-0.08971500
C	-4.46106200	1.37337200	-0.06874300
C	-3.61423300	0.26625300	0.14650100
C	-4.20359200	-0.99796200	0.36393200
C	-5.58232500	-1.14633700	0.34446900
H	-7.48430000	-0.16098400	0.10249200
H	-6.47963500	2.08010900	-0.26229700
H	-4.01529800	2.35273300	-0.22901000
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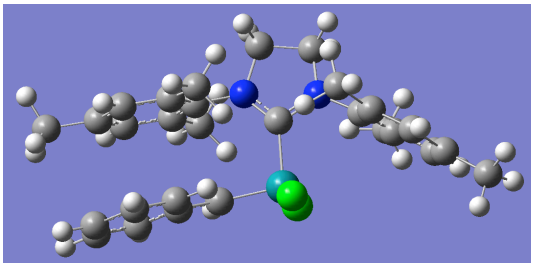
H	-6.02231000	-2.12373900	0.51951100

2Ba TS



Energy: -2210.465925

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C	4.64964000	2.89338500	-0.14744900
C	4.72171700	1.93682400	-1.15955400
C	3.58884800	1.21109500	-1.50207400
C	2.35367300	1.42836200	-0.84819200
C	2.30296600	2.40704800	0.16807100
C	3.43854700	3.12496600	0.51083600
C	-0.59289900	-0.87046900	0.38563800
N	0.36744300	-1.73661300	0.79657600
C	-0.15734400	-2.69650700	1.78044900
C	-1.66582200	-2.53974700	1.63379500
N	-1.76984600	-1.25347000	0.94463900
C	-5.34746000	0.82062500	0.11391400
C	-4.96961900	-0.26943800	-0.66930200
C	-3.81122200	-1.00764000	-0.40445000
C	-3.00755900	-0.59228300	0.66910000
C	-3.38866400	0.46242600	1.51926100
C	-4.55725100	1.15577700	1.21902500
C	4.53670100	-1.14322800	0.66075900
C	3.74853700	-0.45650700	1.58921100
C	2.36545500	-0.62244200	1.64032400
C	1.77404200	-1.51160500	0.72847900
C	2.52842900	-2.21696900	-0.22068100
C	3.90953000	-2.01205500	-0.23598500
C	-3.49994400	-2.23763000	-1.19776100
C	-2.55322200	0.81752600	2.70817300
C	-6.56808100	1.62259300	-0.21789300
C	1.51892800	0.18516000	2.57358600
C	1.85623400	-3.11736100	-1.20667500
C	6.02045400	-0.94370500	0.62718600
H	1.53125800	-0.10541500	-2.05373400
H	5.53479700	3.46194200	0.12661700
H	5.66136900	1.75416800	-1.67455500
H	3.63817800	0.45531100	-2.28368100
H	1.35663800	2.59958200	0.66317400
H	3.38243500	3.87687300	1.29342600
H	0.19759400	-3.70643400	1.55346500
H	0.19617600	-2.43467500	2.78853000
H	-2.11094400	-3.33640600	1.02073800
H	-2.19554600	-2.51000800	2.59146500
H	-5.59272400	-0.56241100	-1.51301700
H	-4.85063700	1.98935100	1.85515800
H	4.21796300	0.25421100	2.26854700
H	4.50969300	-2.53684200	-0.97848500
H	-2.42979400	-2.45070000	-1.23783300
H	-4.01333900	-3.10661100	-0.76573200
H	-3.84092200	-2.13782200	-2.23059800
H	-3.03512200	1.59383000	3.30643500
H	-2.37741100	-0.05247100	3.35238600
H	-1.57500000	1.19840700	2.39726100

H	-7.15741800	1.84928600	0.67575700
H	-6.29463400	2.58344400	-0.66798500
H	-7.21436100	1.10092400	-0.92825500
H	0.81993200	0.82281100	2.01350500
H	0.90435500	-0.44001600	3.23208000
H	2.13373900	0.83201800	3.20378800
H	2.58532800	-3.59736500	-1.86355000
H	1.27961000	-3.90634100	-0.71062700
H	1.13986600	-2.56213000	-1.82693800
H	6.43445500	-1.16685900	-0.36042300
H	6.28895100	0.08571000	0.88332700
H	6.52789600	-1.59737900	1.34607100
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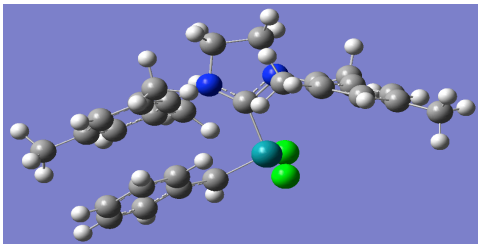
Cl	-0.81058100	-0.97171500	-2.77560600

2Ba local minimum



Energy:

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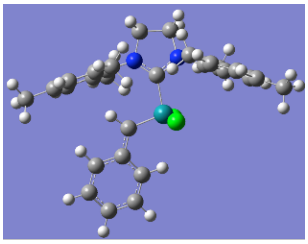
C	4.49730700	2.17477400	-0.96954100
C	3.46019700	1.41689600	-1.49442400
C	2.17710500	1.43055100	-0.90339100
C	1.97250300	2.24662200	0.22997700
C	3.00865800	3.01319400	0.74208700
C	-0.48761800	-0.82093500	0.44130000
N	0.51424700	-1.58005300	0.95761500
C	0.03977100	-2.40838900	2.07742600
C	-1.47356300	-2.35920600	1.91751700
N	-1.64291100	-1.18873500	1.05724700
C	-5.28327000	0.80515000	0.31096900
C	-5.00296900	-0.40374000	-0.32475400
C	-3.82209800	-1.11362800	-0.08368900
C	-2.89622400	-0.54922500	0.80749400
C	-3.16661900	0.64318600	1.50531100
C	-4.36213000	1.30197400	1.23955500
C	4.66803600	-1.01261200	0.45537700
C	3.97070700	-0.33776500	1.45753100
C	2.59931700	-0.51354100	1.64648500
C	1.91720300	-1.38329100	0.78212300
C	2.58968600	-2.10631400	-0.21696200
C	3.96225500	-1.89765000	-0.36316900
C	-3.59806000	-2.45315500	-0.71222500
C	-2.17721200	1.18511800	2.48791200
C	-6.53430400	1.56751200	0.00040100
C	1.88941200	0.22915100	2.73698200
C	1.85912200	-3.05975500	-1.10542700
C	6.13694100	-0.79267400	0.26314600
H	1.40980200	0.23689600	-2.50412200
H	5.08160400	3.57986500	0.55661500
H	5.48021100	2.14607600	-1.43299000
H	3.62468300	0.79244400	-2.37071300
H	0.98248800	2.28186400	0.67659400
H	2.83218900	3.64865100	1.60630600
H	0.45356400	-3.41799000	1.99810900
H	0.37133700	-1.97833200	3.03366000
H	-1.87119200	-3.25750300	1.42370600
H	-2.00739700	-2.22373600	2.86365400
H	-5.72251200	-0.81430600	-1.03145100
H	-4.57255700	2.23808100	1.75458000
H	4.50078200	0.36840200	2.09579900
H	4.49175700	-2.43890800	-1.14639000
H	-2.54102900	-2.64880900	-0.90873600
H	-3.98220100	-3.25139800	-0.06387000
H	-4.12277500	-2.53040900	-1.66716500
H	-2.57512900	2.06240200	3.00259700
H	-1.90099700	0.43780500	3.24201700
H	-1.25596100	1.49092300	1.97757800

H	-7.01540400	1.94150000	0.90940100
H	-6.31480900	2.44107000	-0.62343800
H	-7.25906600	0.95324900	-0.53989700
H	0.86435300	0.49268500	2.45638800
H	1.83335800	-0.36273100	3.65927000
H	2.41805100	1.15413100	2.98204700
H	2.55838100	-3.67679500	-1.67467700
H	1.20177600	-3.72429800	-0.53426000
H	1.20537200	-2.53660800	-1.81289500
H	6.40820300	-0.79907700	-0.79723100
H	6.45585700	0.16345500	0.68825300
H	6.72767900	-1.57837300	0.74798500
Cl	-1.32456900	2.60836700	-0.52414500
Cl	-0.93083700	-1.42236700	-2.63232100

2Bi



Energy: -2210.473504

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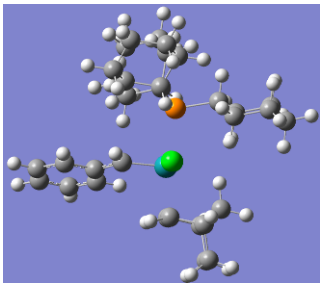
Cl	0.31520600	1.30415100	2.34521100
C	-1.58858000	0.91293700	-0.27671900
H	-2.15488900	0.03959200	-0.61303900
C	-3.96145200	4.43596300	-0.09165200
C	-4.49783900	3.24151600	-0.57395200
C	-3.71114600	2.09892600	-0.62142100
C	-2.36707700	2.12578300	-0.19095500
C	-1.84645800	3.34145000	0.30290200
C	-2.63608300	4.48052800	0.34737900
C	0.56578200	-1.06132400	0.27244400
N	-0.27585900	-2.10018200	0.52458600
C	0.44817300	-3.36388800	0.72100400
C	1.88916800	-2.90382100	0.89992000
N	1.83602300	-1.52233600	0.41997100
C	5.29880800	0.72217200	-0.45914700
C	4.81839500	0.65728100	0.84723500
C	3.68917800	-0.09640900	1.18843200
C	3.01855800	-0.76445500	0.15422200
C	3.50902600	-0.77204500	-1.16538000
C	4.64397500	-0.01990500	-1.44860000
C	-4.38388900	-2.18755600	-0.41763300
C	-3.41774300	-2.33456700	-1.41939100
C	-2.05325000	-2.31141300	-1.13133800
C	-1.66546700	-2.14408700	0.20786900
C	-2.59998800	-1.99039500	1.23828600
C	-3.95620000	-2.01610100	0.89986800
C	3.28517500	-0.23001500	2.62379900
C	2.82056200	-1.57384000	-2.22421000
C	6.48382600	1.57090400	-0.80414900
C	-1.03358100	-2.33802200	-2.22706700
C	-2.14619300	-1.73525200	2.64013700
C	-5.84241900	-2.19251900	-0.76168100
H	-4.57617500	5.33088900	-0.05276400
H	-5.53038000	3.20455100	-0.91009600
H	-4.12035000	1.16148100	-0.99433300
H	-0.82400200	3.37576600	0.67623800
H	-2.22319600	5.40865700	0.73166300
H	0.05168300	-3.89766300	1.59045400
H	0.31779600	-4.01157700	-0.15827700
H	2.21261400	-2.92588700	1.95012600
H	2.60746000	-3.48727200	0.31395100
H	5.33960100	1.19961800	1.63492900
H	5.02042500	-0.00071100	-2.47020800
H	-3.73402200	-2.44942000	-2.45566800
H	-4.69640900	-1.88316800	1.68738700
H	3.97365600	-0.90575400	3.14676700
H	3.32214600	0.73370800	3.13801300
H	2.26988100	-0.61141400	2.74121800
H	3.34164800	-1.48976300	-3.18038600
H	2.76929000	-2.63786400	-1.95969900

H	1.79473200	-1.22108400	-2.37198800
H	7.13065100	1.08234000	-1.53884300
H	6.16755000	2.52352800	-1.24389300
H	7.08550000	1.80430500	0.07805400
H	-0.58132700	-1.34430000	-2.35728100
H	-0.20710200	-3.02652200	-2.02011500
H	-1.48304200	-2.62617600	-3.18000300
H	-2.99534000	-1.65868900	3.32277900
H	-1.48742700	-2.52979900	3.00793800
H	-1.56854400	-0.80450700	2.70013300
H	-6.46706500	-2.11096100	0.13100500
H	-6.09923200	-1.35792900	-1.42371300
H	-6.12857500	-3.10861900	-1.28865400

1Ca



Energy: -2605.023964

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Ru	-1.18186500	0.01404300	0.29623300
Cl	-1.19732100	0.44907100	-2.14929500
H	-0.30289200	1.61658600	2.02989800
P	1.19758600	-0.57725300	-0.11797600
C	2.29177400	-0.52125100	1.38659000
C	2.01121400	0.35985300	-1.49461700
C	1.27471000	-2.35286900	-0.65869300
C	3.51792700	-1.44440800	1.40333900
C	4.16244700	-1.42398000	2.78878300
C	4.54265000	-0.01121200	3.21536800
C	3.34312900	0.92672400	3.14901400
C	2.71231500	0.90457800	1.76027000
C	3.47617100	-0.00306400	-1.75301100
C	3.95835000	0.64658100	-3.04825900
C	3.77087800	2.15933600	-3.01085100
C	2.32429600	2.53160400	-2.70273600
C	1.83911700	1.88042300	-1.41107900
C	0.67162300	-3.27122200	0.41290300
C	0.77915700	-4.73693400	0.01014800
C	0.11832400	-4.98469500	-1.33978500
C	0.71562400	-4.07763700	-2.40800500
C	0.61189500	-2.60685500	-2.01677900
H	1.60918800	-0.87032200	2.17596800
H	1.42106100	0.04572900	-2.36732600
H	2.34575200	-2.59381500	-0.75958000
H	3.24567000	-2.47449100	1.15022900
H	4.25459100	-1.12126300	0.65493600
H	5.04090300	-2.07986700	2.80174500
H	3.44996600	-1.84299700	3.51419200
H	5.33126800	0.36711700	2.54726500
H	4.97126300	-0.01801400	4.22417200
H	3.63857200	1.94887700	3.41358500
H	2.58899600	0.61636400	3.88660700
H	3.44592100	1.27501500	1.02838000
H	1.85729600	1.59068100	1.71398500
H	4.09776400	0.35874300	-0.92063200
H	3.61659300	-1.09091500	-1.79747500
H	3.38649800	0.22908000	-3.89018900
H	5.00910300	0.39114200	-3.22980700
H	4.09204900	2.60751300	-3.95831300
H	4.42536200	2.58118900	-2.23279600
H	1.67406200	2.20064300	-3.52581600
H	2.21121600	3.62027700	-2.63803400
H	0.78684300	2.12354000	-1.23937600
H	2.40867900	2.28468800	-0.56310500
H	1.13844800	-3.10064000	1.39034700
H	-0.38446900	-3.00110300	0.56174100
H	0.33296300	-5.37068800	0.78487600
H	1.84160600	-5.02023000	-0.04753800

H	-0.95956400	-4.77902100	-1.25451200
H	0.21052200	-6.03757500	-1.63050700
H	0.22494400	-4.23983600	-3.37454000
H	1.77508900	-4.33933600	-2.55233400
H	-0.44474500	-2.30604800	-1.97284500
H	1.05983200	-1.97975200	-2.79623800
C	-3.39269000	0.33689000	-0.13871400
C	-3.27565000	-0.15491500	1.16090200
H	-3.52457800	1.37997300	-0.41484100
C	-3.92615300	-0.80369700	-0.98209100
H	-3.29310000	0.43163500	2.07374000
C	-3.72055400	-1.60160500	1.11974400
C	-3.25890200	-1.99933200	-0.28862800
C	-5.25531000	-1.55925600	0.90779900
C	-5.39631800	-1.00303400	-0.53179600
H	-3.77064500	-0.70279300	-2.05666900
H	-3.37297100	-2.21539800	1.95242000
H	-3.64136100	-2.97215500	-0.61829800
H	-2.15950600	-2.02970100	-0.41072100
H	-5.67525400	-2.56789000	0.98909100
H	-5.90303100	-1.71669000	-1.19059600
H	-5.75585800	-0.94043500	1.65880100
H	-5.96268800	-0.06761500	-0.57409400
C	-0.53619300	4.07549300	1.46458100
H	-0.06221100	3.79903900	2.40489300
C	-0.68209500	5.41225600	1.12079800
H	-0.32505400	6.18878900	1.79155000
C	-1.28734200	5.75327300	-0.08933300
H	-1.40201700	6.79887700	-0.36297700
C	-1.74428200	4.75201300	-0.94969100
H	-2.21083500	5.02037900	-1.89365900
C	-1.60277300	3.41408700	-0.61073700
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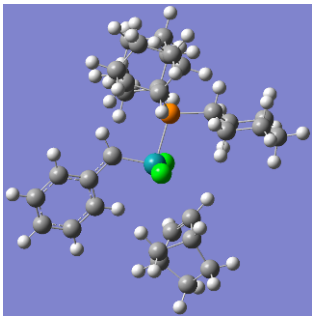
C	-0.99057500	3.04732000	0.60742200

1Ci



Energy: -2605.0105

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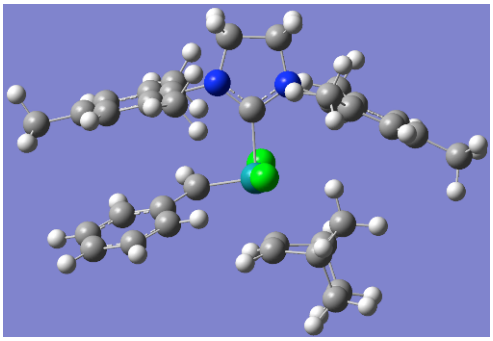
Ru	0.75619100	-0.05327200	-0.05766300
Cl	0.78498600	-0.04913500	-2.46796100
H	-0.18043700	-2.41979000	0.63253400
P	-1.50822100	0.20342100	-0.03997700
C	-2.38632900	-0.12613900	1.57897600
C	-2.38386800	-0.66143300	-1.43180300
C	-1.87761500	2.00461200	-0.34028000
C	-3.69790200	0.64070200	1.81610000
C	-4.22251400	0.38894300	3.22793500
C	-4.42539200	-1.09602700	3.49390400
C	-3.13349700	-1.86382100	3.25418900
C	-2.59454400	-1.62081100	1.84788200
C	-3.90792200	-0.50390500	-1.43483400
C	-4.50345100	-1.05756400	-2.72649800
C	-4.11399100	-2.51622200	-2.93037600
C	-2.59960700	-2.68257500	-2.90750800
C	-1.98413800	-2.12744500	-1.62692500
C	-1.26199000	2.87569900	0.76092500
C	-1.69241100	4.32827300	0.60960900
C	-1.31364400	4.87006100	-0.76344900
C	-1.88059000	3.99336600	-1.87407800
C	-1.45673200	2.53553400	-1.71325000
H	-1.65001200	0.23939000	2.31173600
H	-1.98022900	-0.12609600	-2.30488100
H	-2.97492600	2.08946900	-0.27689000
H	-3.55581600	1.71665900	1.67644400
H	-4.46022500	0.32950700	1.08926700
H	-5.15651800	0.94243800	3.37977500
H	-3.50074100	0.79267700	3.95279100
H	-5.20670700	-1.48114000	2.82121900
H	-4.78853900	-1.26000100	4.51481900
H	-3.28461100	-2.93761800	3.41411500
H	-2.37690700	-1.54315200	3.98435400
H	-3.30372500	-2.03243200	1.11373000
H	-1.65548800	-2.16819000	1.71898900
H	-4.33481800	-1.05138500	-0.58136100
H	-4.19658400	0.54730300	-1.30594700
H	-4.13616000	-0.46044600	-3.57407100
H	-5.59371300	-0.94347700	-2.71544200
H	-4.52957400	-2.89751000	-3.87000900
H	-4.55907600	-3.12226300	-2.12669900
H	-2.16085200	-2.14904600	-3.76320900
H	-2.32380800	-3.73639500	-3.02756600
H	-0.89318900	-2.20252700	-1.68059900
H	-2.31430500	-2.73124200	-0.76793200
H	-1.50474400	2.49562900	1.75994600
H	-0.16588700	2.80585100	0.69659900

H	-1.24559300	4.93659700	1.40403200
H	-2.78320800	4.39858200	0.74218000
H	-0.21675300	4.89284000	-0.84850300
H	-1.65335500	5.90566300	-0.87906100
H	-1.56759700	4.36420000	-2.85660100
H	-2.97951900	4.05359900	-1.85760900
H	-0.36578400	2.45243000	-1.81879600
H	-1.87578100	1.92854900	-2.52413400
C	2.76617300	1.86149600	-0.26878800
C	3.52996800	1.02153000	-1.00183600
H	1.85373100	2.35963500	-0.60840100
C	3.56035800	2.23789100	0.95876000
H	3.31803900	0.67668300	-2.00934300
C	4.82237500	0.82831200	-0.25252200
C	4.32453700	0.92717300	1.19619200
C	5.58577100	2.17922400	-0.38330600
C	4.71390600	3.14894700	0.44847400
H	2.98563000	2.63558300	1.79609200
H	5.41493200	-0.04889000	-0.52606800
H	5.13580300	1.02464600	1.92667200
H	3.66013300	0.10580000	1.48834400
H	6.59139900	2.08188400	0.03967300
H	5.27164200	3.55707200	1.29790100
H	5.69926300	2.48821600	-1.42663200
H	4.34247300	3.99696000	-0.13438800
C	1.89905600	-3.93137000	0.93211300
H	1.01817400	-4.20611300	1.50902800
C	3.02288500	-4.74627700	0.93894000
H	3.02422800	-5.66398100	1.52057800
C	4.14777500	-4.38801900	0.19464600
H	5.02510600	-5.02883500	0.19327100
C	4.14143100	-3.21052900	-0.55587600
H	5.01103400	-2.94010500	-1.14899800
C	3.02444600	-2.38682400	-0.55626700
H	2.99948800	-1.48275300	-1.16164300
C	1.88329200	-2.72632900	0.19795300

2Ca



Energy: -2483.277684

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N	1.03609300	-2.26713300	0.12732300
C	0.75355400	-3.68522900	0.41428100
C	-0.76847000	-3.72517800	0.48638500
C	-2.49680500	-1.89204100	0.35834300
C	2.39861200	-1.85927600	-0.00745600
C	-3.03551100	-1.56301200	1.61729000
C	-4.34041000	-1.07212300	1.66013900
C	-5.12135300	-0.94519000	0.50840100
C	-4.58622100	-1.37643200	-0.70554800
C	-3.28361500	-1.87294300	-0.80688900
C	3.01210200	-1.95722000	-1.26739100
C	4.35491900	-1.59174100	-1.37004400
C	5.08712000	-1.15296200	-0.26311400
C	4.44847100	-1.09502000	0.97630900
C	3.10747400	-1.45042500	1.13242400
C	-2.29061100	-1.80757800	2.89357200
H	-4.75842500	-0.78553600	2.62454800
C	-6.49665300	-0.35637600	0.57912500
H	-5.19863500	-1.33205300	-1.60537200
C	-2.80445200	-2.43813600	-2.10791600
C	2.23241200	-2.39416400	-2.46557800
H	4.83793900	-1.64276800	-2.34550600
C	6.52534200	-0.75892600	-0.40519900
H	5.00147400	-0.74482600	1.84718800
C	2.43683100	-1.35035500	2.46309700
H	-2.45485000	-0.99701100	3.60689300
H	-1.21209400	-1.88184900	2.74539700
H	-2.64638200	-2.73651200	3.35866300
H	-6.45449600	0.73946900	0.59242300
H	-7.02280600	-0.66231700	1.48810000
H	-7.10571400	-0.64480400	-0.28149000
H	-3.02883100	-1.76762000	-2.94076100
H	-3.31002900	-3.39234200	-2.30434400
H	-1.72619200	-2.60181200	-2.12353600
H	2.87720000	-2.48481300	-3.34277000
H	1.42788600	-1.68313600	-2.69744400
H	1.74489000	-3.36342700	-2.30674900
H	6.83763700	-0.08761600	0.39967800
H	6.70970300	-0.25351700	-1.35858200
H	7.18545700	-1.63347400	-0.37584100
H	3.16212500	-1.13838500	3.25240100
H	1.90725300	-2.27311600	2.72893500
H	1.67948900	-0.55618300	2.46782400
H	1.23891500	-3.97540800	1.35436800
H	-1.14658500	-4.07350400	1.45499800
H	1.16544300	-4.31765100	-0.38072900

H	-1.22241500	-4.34669700	-0.29540600
Ru	-0.31594100	0.57110600	-0.27757400
Cl	-0.44632700	0.74492400	2.19410100
Cl	-0.57498900	-0.09955600	-2.65589400
C	1.48200100	0.90347000	-0.66772600
H	1.80343600	0.49040000	-1.63865600
C	-0.92251300	2.79721100	0.05014600
C	-1.07751800	2.50782800	-1.29621900
C	-2.31640400	2.89083100	0.63445300
H	-0.05595700	3.26848400	0.50730200
C	-2.56483900	2.40050700	-1.55232000
H	-0.36130200	2.70907500	-2.08641400
C	-3.04858000	1.84113500	-0.20912800
C	-2.92500600	4.19215100	0.04602500
C	-3.09706400	3.85384900	-1.45731100
H	-2.37910200	2.78730500	1.71852400
H	-2.84530800	1.85067000	-2.45296800
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H	-2.72745600	0.80571000	-0.00822300
H	-2.28160600	5.06060000	0.21819300
H	-3.88925900	4.40572400	0.52029800
H	-2.54783500	4.53432200	-2.11538400
H	-4.14969200	3.89288200	-1.75839300
C	3.73076100	1.86195100	-0.73907500
H	3.82329000	1.42187600	-1.73029600
C	4.78637600	2.57662400	-0.18777600
H	5.70639100	2.70909800	-0.75166300
C	4.66590100	3.11290700	1.09438100
H	5.49289300	3.66654100	1.53183100
C	3.48045800	2.94203700	1.81331600
H	3.38673800	3.36145600	2.81143200
C	2.41599700	2.24446000	1.26019900
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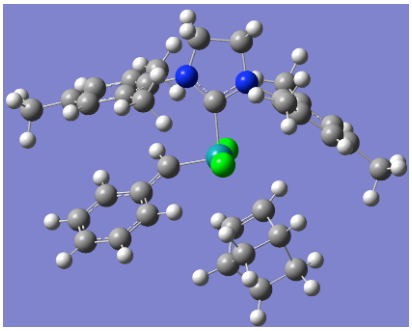
2Ci



Energy: -2483.268452

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C	1.06443700	-3.78902800	0.80291100
C	-0.45156200	-3.94757400	0.75568200
C	-2.26610700	-2.17651500	0.43515400
C	2.58218200	-1.91052700	0.10651700
C	-2.99706500	-1.70764900	1.54233200
C	-4.26243300	-1.16629100	1.30468800
C	-4.81933700	-1.12037200	0.02536800
C	-4.11817200	-1.71746300	-1.02575100
C	-2.84909300	-2.27005600	-0.84433100
C	3.18414100	-2.08020600	-1.14875000
C	4.47623800	-1.58124500	-1.32633500
C	5.16045900	-0.92827500	-0.29771800
C	4.52759800	-0.78596900	0.94004500
C	3.23872800	-1.26929300	1.16805600
C	-2.48550100	-1.84334100	2.94149400
H	-4.82038900	-0.75700200	2.14613700
C	-6.12606400	-0.42984100	-0.21687200
H	-4.56261200	-1.74643900	-2.01979600
C	-2.18639900	-3.01319100	-1.96269600
C	2.42890100	-2.71187800	-2.27472300
H	4.95584600	-1.69901800	-2.29725200
C	6.52785800	-0.35974600	-0.52420100
H	5.04440600	-0.27129900	1.74920400
C	2.55558100	-1.07175400	2.48239900
H	-2.76240300	-0.98009400	3.55023500
H	-1.39823800	-1.92762600	2.97588300
H	-2.92090500	-2.73666200	3.40876700
H	-5.96622000	0.63656000	-0.42081600
H	-6.78640600	-0.49171500	0.65265600
H	-6.65355700	-0.84596800	-1.07936300
H	-2.46640000	-2.59827500	-2.93253600
H	-2.49980800	-4.06575200	-1.94403600
H	-1.09692500	-2.97642000	-1.90920900
H	3.07260400	-2.86929800	-3.14324600
H	1.58599000	-2.07610900	-2.58139700
H	1.99807500	-3.67963400	-1.99252200
H	6.47773300	0.71634800	-0.73089900
H	7.02671200	-0.82973400	-1.37576300
H	7.16739800	-0.48097900	0.35485200
H	3.23308700	-0.62951700	3.21622700
H	2.17884100	-2.01424100	2.89720100
H	1.68248200	-0.41458800	2.38204200
H	1.46373000	-3.86820700	1.82373000
H	-0.86762500	-4.39573500	1.66397000
H	1.59920400	-4.51003300	0.17618200

H	-0.78475000	-4.54481200	-0.10528400
Ru	-0.38729600	0.18306200	-0.18199300
Cl	-0.64449200	0.65653300	2.20430000
Cl	-0.48691300	-0.36004000	-2.60082400
C	1.35658700	0.79375700	-0.50223000
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C	-1.25355600	2.47346700	-1.25595700
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C	-1.35475100	3.84470300	-0.64043300
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H	-0.46711300	4.47792400	-0.70928900
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H	-2.60609900	4.40393100	-2.38628600
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H	-4.36764100	3.07123200	-1.44235200
H	-4.46285100	4.20498700	-0.09293400
C	3.36297800	2.17809500	-0.66367700
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C	3.74664500	4.07365300	0.77154400
H	4.36875900	4.90974200	1.08031500
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H	2.21798600	4.46885900	2.23883400
C	1.72803000	2.76936200	1.02545900
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