Supplementary Materials: Olefin Metathesis with Ru-based Catalysts Exchanging the Typical *N*-Heterocyclic Carbenes by a Phosphine–Phosphonium Ylide

Laia Arnedo, Remi Chauvin and Albert Poater

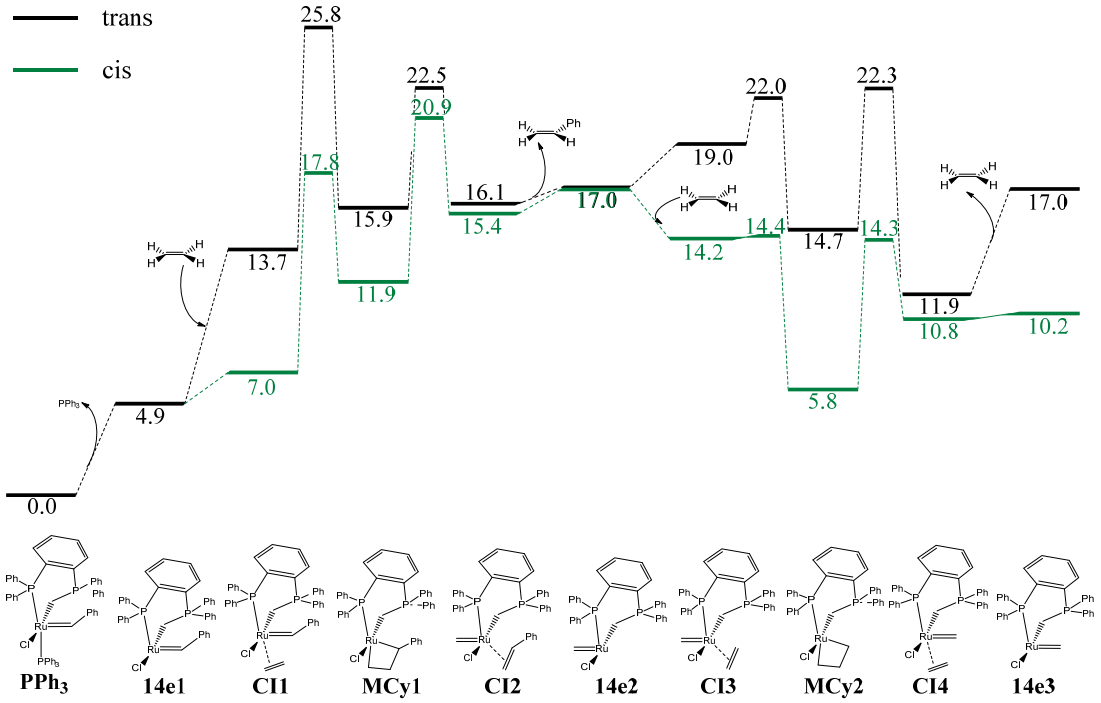


Figure S1. Free-energy profile in solvent for the olefin metathesis reaction of complex **A** using ethylene as the substrate (energies in kcal/mol calculated at *P* = 1 atm (instead of 1354).

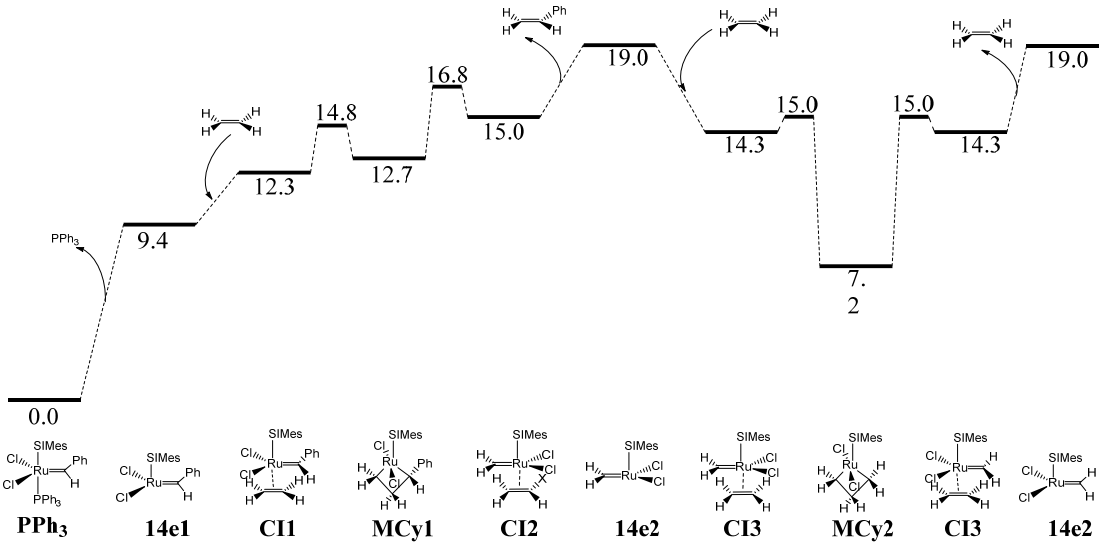
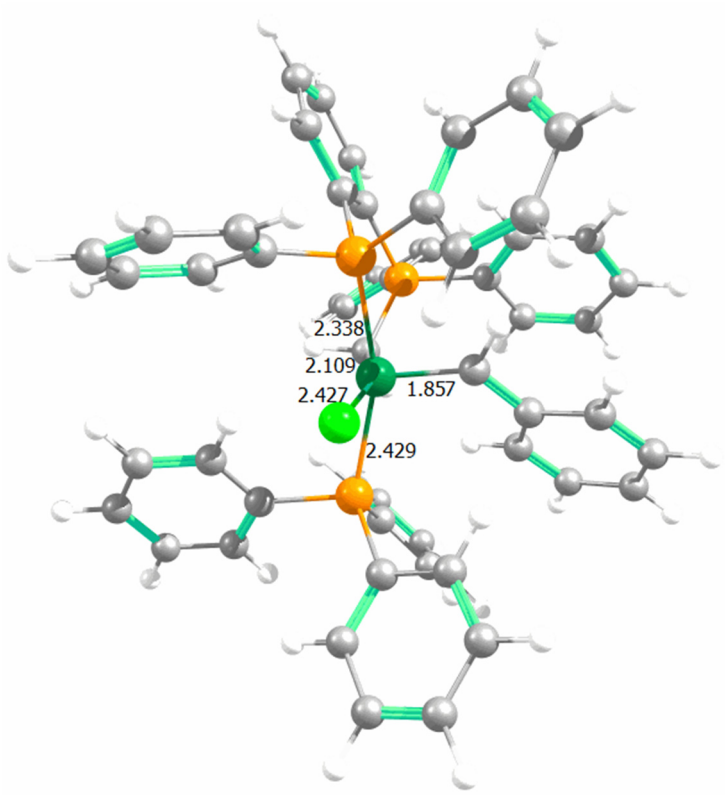


Figure S2. Free-energy profile in solvent for the olefin metathesis reaction of complex **B** using ethylene as the substrate (energies in kcal/mol calculated at *P* = 1 atm (instead of 1354), SIMes = 1,3-Bis(2,4,6-trimethylphenyl)-4,5-dihydroimidazol-2-ylidene).

Table S1. 3D view and *xyz* coordinate data sets and absolute energies in a.u. for DFT optimized complexes.

A-PPh_3



Zero-point correction = 0.838172 (Hartree/Particle)

Thermal correction to Energy = 0.894279

Thermal correction to Enthalpy = 0.895223

Thermal correction to Gibbs Free Energy = 0.745534

Sum of electronic and zero-point Energies = −3738.930127

Sum of electronic and thermal Energies = −3738.874020

Sum of electronic and thermal Enthalpies = −3738.873076

Sum of electronic and thermal Free Energies = −3739.022765

P	-1.905184	-1.611442	0.131275
P	-1.842636	1.738355	-0.815461
C	-0.266352	0.916271	-1.114870
C	-3.258061	0.625203	-1.159920
C	-4.363255	1.178438	-1.851833
C	-5.475073	0.389829	-2.178716
C	-5.490043	-0.972236	-1.835446
C	-4.394956	-1.531049	-1.161620
C	-3.274478	-0.749175	-0.793609
C	0.032419	0.111056	1.783006
C	-2.670748	-2.010202	1.766567
C	-3.995115	-1.662857	2.117627
C	-4.473721	-1.917639	3.414686
C	-3.641959	-2.526796	4.370535
C	-2.324540	-2.877831	4.025381
C	-1.833286	-2.614705	2.736015
C	-1.826892	-3.182427	-0.831355
C	-1.944249	-4.453789	-0.239010
C	-1.763312	-5.606979	-1.022732
C	-1.464921	-5.497126	-2.392013
C	-1.350032	-4.226273	-2.985488
C	-1.525690	-3.071349	-2.207991
C	-2.013690	3.196219	-1.907822
C	-1.347904	3.206636	-3.153848
C	-1.488168	4.307751	-4.014578
C	-2.289802	5.400176	-3.638423
C	-2.952853	5.394217	-2.397622
C	-2.817414	4.297693	-1.531015
C	-1.953519	2.364152	0.886606
C	-2.691453	1.661629	1.862267
C	-2.660262	2.084581	3.199493
C	-1.905964	3.214635	3.562337
C	-1.191948	3.931606	2.585870
C	-1.207115	3.507694	1.248322
H	0.470007	1.750113	-1.096475
H	-4.349386	2.236003	-2.153244
H	-6.323999	0.840447	-2.715395
H	-6.353410	-1.603680	-2.096525
H	-4.402788	-2.602450	-0.906678
H	-0.768426	-0.320635	2.426948
H	-4.665700	-1.189464	1.384479
H	-5.507927	-1.642762	3.675321
H	-4.021760	-2.729095	5.384233
H	-1.666761	-3.358631	4.766408
H	-0.795876	-2.879787	2.470342
H	-2.170711	-4.547343	0.833533
H	-1.853576	-6.600093	-0.555896
H	-1.323832	-6.404290	-2.999877
H	-1.127180	-4.133016	-4.059945
H	-1.429681	-2.077456	-2.677235
H	-0.714829	2.358660	-3.457115
H	-0.966614	4.312158	-4.984136
H	-2.396689	6.262635	-4.314592
H	-3.578273	6.250204	-2.100373
H	-3.332844	4.300241	-0.557816
H	-3.278771	0.775542	1.586712
H	-3.222455	1.518410	3.957826
H	-1.872473	3.540123	4.613244
H	-0.594049	4.809771	2.871324
H	-0.627265	4.058575	0.491271
Ru	0.250453	-0.706249	0.130242
C	0.796439	1.124921	2.501511
C	0.748879	1.106066	3.924053
C	1.539525	2.151888	1.869027
C	1.457495	2.049990	4.678750
H	0.151652	0.328032	4.426864
C	2.235007	3.104338	2.622874
H	1.539333	2.210580	0.774547
C	2.204032	3.052677	4.029441
H	1.425465	2.010561	5.778834
H	2.805540	3.891610	2.106619
H	2.756779	3.798584	4.622003
Cl	1.047347	-2.905385	0.778764
P	2.580319	-0.337071	-0.448727
C	3.241839	1.354323	-0.812361
C	2.739180	2.089232	-1.914760
C	4.176156	1.970876	0.048854
C	3.136277	3.419817	-2.126962
H	2.066394	1.603581	-2.638167
C	4.579127	3.298801	-0.173600
H	4.582870	1.412332	0.905416
C	4.052320	4.031604	-1.251618
H	2.739248	3.976844	-2.990259
H	5.314483	3.762429	0.502771
H	4.368908	5.072534	-1.421593
C	3.863168	-1.043889	0.665301
C	5.099143	-1.506517	0.167559
C	3.617709	-1.054332	2.054602
C	6.084221	-1.968191	1.056581
H	5.293600	-1.516695	-0.915885
C	4.610368	-1.506005	2.939079
H	2.645446	-0.718292	2.440996
C	5.843781	-1.963929	2.442331
H	7.044531	-2.336387	0.662771

	H	4.412912	-1.511012	4.022416
	H	6.618168	-2.326315	3.136576
	C	2.795701	-1.171776	-2.098713
	C	3.786991	-0.737991	-3.012218
	C	1.957570	-2.250262	-2.467741
	C	3.929711	-1.363720	-4.261786
	H	4.454110	0.097539	-2.750321
	C	2.098200	-2.865729	-3.722846
	H	1.212613	-2.652643	-1.763962
	C	3.081637	-2.425533	-4.624367
	H	4.711564	-1.017884	-4.956204
	H	1.435347	-3.705454	-3.983729
	H	3.193916	-2.912688	-5.605721
	H	-0.310655	0.523356	-2.159018

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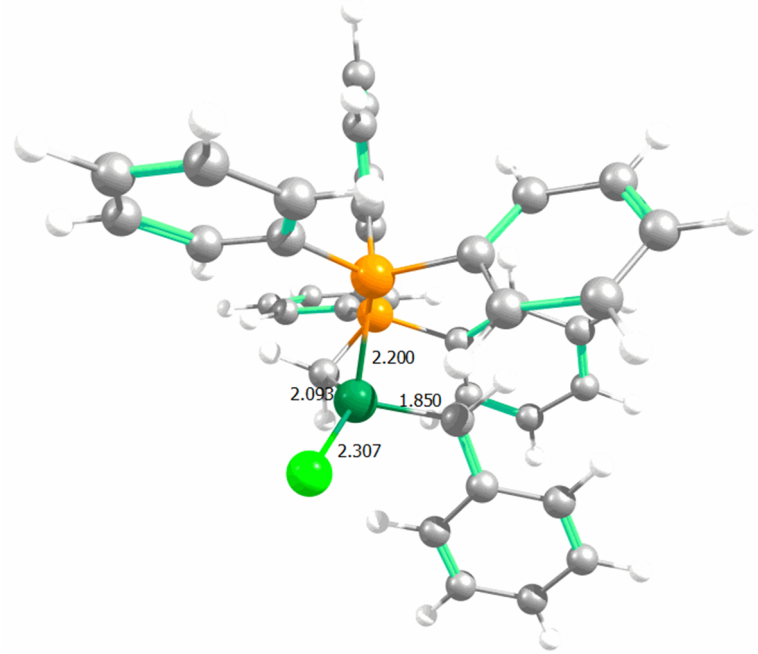

Zero-point correction = 0.568783 (Hartree/Particle)
Thermal correction to Energy = 0.607717
Thermal correction to Enthalpy = 0.608661
Thermal correction to Gibbs Free Energy = 0.494413
Sum of electronic and zero-point Energies = −2703.363947
Sum of electronic and thermal Energies = −2703.325013
Sum of electronic and thermal Enthalpies = −2703.324069
Sum of electronic and thermal Free Energies = −2703.438317

P	1.748353	-0.371426	0.140240
P	-1.643328	-1.241347	-0.099226
C	-0.898175	-0.656821	-1.630905
C	-0.414808	-2.185022	0.882280
C	-0.892946	-3.321331	1.579323
C	-0.022140	-4.122427	2.331907
C	1.347077	-3.813014	2.379881
C	1.832533	-2.696268	1.683909
C	0.966450	-1.854592	0.948323
C	-0.130185	1.939757	-0.271351
C	2.265860	0.702550	1.544984
C	1.972332	0.412094	2.894295
C	2.339693	1.320627	3.903153
C	3.001309	2.515706	3.571760
C	3.293399	2.808300	2.226207
C	2.919895	1.913558	1.211659
C	3.277822	-1.109758	-0.569817
C	4.571864	-0.736497	-0.155282
C	5.693859	-1.296879	-0.791573
C	5.529304	-2.221670	-1.836754
C	4.236519	-2.597475	-2.248700
C	3.113363	-2.043115	-1.618840
C	-3.046637	-2.367925	-0.416965
C	-2.985756	-3.241966	-1.525856
C	-4.033498	-4.145978	-1.762298
C	-5.141181	-4.184226	-0.895830
C	-5.204416	-3.315378	0.208440
C	-4.161715	-2.406527	0.452117
C	-2.306192	0.136749	0.876814
C	-1.725818	0.506384	2.107657
C	-2.245979	1.601511	2.817389
C	-3.339051	2.320253	2.302838
C	-3.917519	1.950179	1.074727
C	-3.405356	0.859864	0.357897
H	-1.721539	-0.216282	-2.239549
H	-1.957014	-3.594905	1.520522
H	-0.415289	-4.999781	2.867897
H	2.041651	-4.444285	2.955400
H	2.908607	-2.462434	1.713045
H	0.211300	2.045615	0.780991
H	1.465552	-0.525592	3.169024
H	2.110749	1.088113	4.954934
H	3.289513	3.223623	4.364472
H	3.808970	3.744607	1.961852
H	3.118276	2.158292	0.154576
H	4.710114	-0.011157	0.660606
H	6.704514	-1.003970	-0.467354
H	6.411721	-2.652026	-2.335090
H	4.104881	-3.321460	-3.067653
H	2.101462	-2.337731	-1.944406
H	-2.123805	-3.220118	-2.211023
H	-3.985369	-4.822579	-2.629333
H	-5.961943	-4.893473	-1.084705
H	-6.072567	-3.342733	0.884967
H	-4.216267	-1.726004	1.315999
H	-0.862386	-0.047888	2.505164
H	-1.788570	1.895151	3.774518
H	-3.740139	3.181780	2.858433
H	-4.759974	2.525754	0.663220
H	-3.859801	0.575938	-0.604303
Ru	0.658693	0.727005	-1.424176
C	-1.103534	2.947522	-0.682406
C	-1.390566	4.013358	0.212884
C	-1.805042	2.900914	-1.919682
C	-2.347363	4.986057	-0.108829
H	-0.854370	4.061038	1.173837
C	-2.762029	3.870430	-2.237753
H	-1.595899	2.091551	-2.638417
C	-3.040347	4.913933	-1.330748
H	-2.556110	5.805530	0.596512
H	-3.295091	3.821167	-3.199965
H	-3.793468	5.676228	-1.584494
Cl	2.368914	1.745105	-2.590873
H	-0.503282	-1.552630	-2.165434

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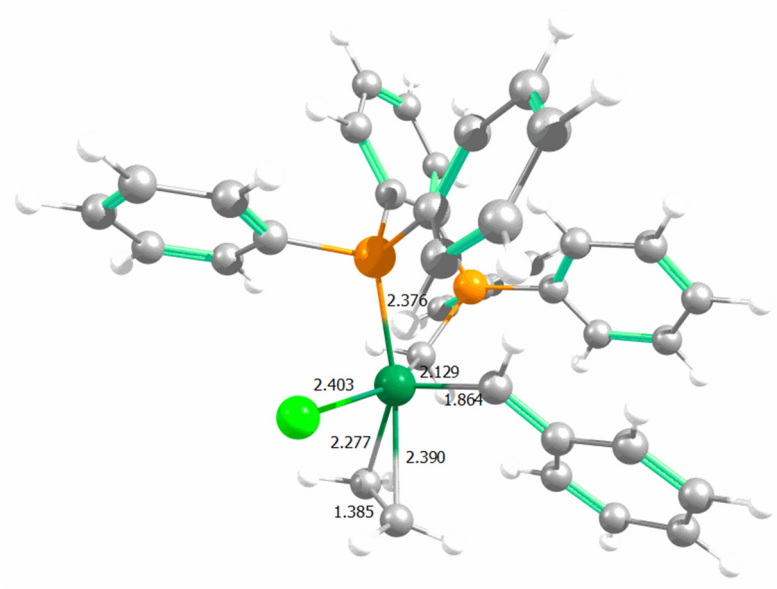

Zero-point correction = 0.622047 (Hartree/Particle)

Thermal correction to Energy = 0.663814

Thermal correction to Enthalpy = 0.664759

Thermal correction to Gibbs Free Energy = 0.547325

Sum of electronic and zero-point Energies = −2781.857411

Sum of electronic and thermal Energies = −2781.815643

Sum of electronic and thermal Enthalpies = −2781.814699

Sum of electronic and thermal Free Energies = −2781.932133

P	1.777757	-0.302669	0.194679
P	-1.534498	-1.385768	-0.047075
C	-0.918904	-0.674449	-1.592512
C	-0.225439	-2.339252	0.805635
C	-0.606312	-3.569139	1.395562
C	0.334860	-4.374054	2.052022
C	1.677552	-3.967209	2.111401
C	2.065449	-2.756011	1.520988
C	1.128836	-1.911040	0.878220
C	-0.336284	1.919151	-0.327330
C	2.127845	0.704742	1.704725
C	1.981040	0.207514	3.019068
C	2.221021	1.044341	4.122940
C	2.617020	2.378909	3.927020
C	2.777054	2.874695	2.620659
C	2.530850	2.048408	1.511832
C	3.414165	-0.875544	-0.427221
C	4.634034	-0.444588	0.126488
C	5.845496	-0.908597	-0.416562
C	5.841028	-1.795993	-1.506022
C	4.619969	-2.226045	-2.059100
C	3.408648	-1.765735	-1.523213
C	-2.908567	-2.542077	-0.391162
C	-2.920397	-3.260622	-1.608112
C	-3.946920	-4.183217	-1.867404
C	-4.961668	-4.395486	-0.917155
C	-4.950907	-3.685158	0.296874
C	-3.929046	-2.759840	0.564338
C	-2.193644	-0.128677	1.087961
C	-1.454376	0.274663	2.219038
C	-1.939174	1.304142	3.040657
C	-3.168604	1.918471	2.745672
C	-3.919079	1.501295	1.631081
C	-3.434138	0.484201	0.796588
H	-1.844751	-0.361166	-2.122916
H	-1.649650	-3.910751	1.328980
H	0.017795	-5.326290	2.504033
H	2.429309	-4.595631	2.613477
H	3.122367	-2.450274	1.559309
H	0.132322	2.018002	0.678582
H	1.680463	-0.836458	3.195435
H	2.104019	0.644853	5.142536
H	2.806893	3.031321	4.793606
H	3.097470	3.915668	2.458288
H	2.661812	2.438672	0.489246
H	4.643233	0.258308	0.973336
H	6.799748	-0.567992	0.014490
H	6.792529	-2.152710	-1.929892
H	4.613479	-2.917789	-2.915731
H	2.452725	-2.098773	-1.962756
H	-2.131860	-3.103624	-2.359928
H	-3.953971	-4.737715	-2.818384
H	-5.766395	-5.117818	-1.124569
H	-5.744811	-3.850423	1.041528
H	-3.926904	-2.206466	1.516123
H	-0.494979	-0.202479	2.458743
H	-1.346155	1.625030	3.910697
H	-3.547224	2.728958	3.387178
H	-4.875670	1.989642	1.393268
H	-4.019237	0.172619	-0.082346
Ru	0.587673	0.827857	-1.522597
C	-1.512804	2.770642	-0.457939
C	-1.656780	3.848603	0.458920
C	-2.558432	2.546378	-1.395833
C	-2.777632	4.689628	0.413773
H	-0.867512	4.019155	1.208535
C	-3.684034	3.376175	-1.429851
H	-2.486847	1.690801	-2.082006
C	-3.794543	4.455525	-0.529597
H	-2.863027	5.529295	1.120910
H	-4.486138	3.184085	-2.159470
H	-4.677938	5.112228	-0.563357
Cl	2.742491	1.767377	-2.022913
C	-0.128629	1.066844	-3.670261
H	-1.131718	0.637452	-3.831436
H	0.700301	0.539598	-4.180297
C	0.030233	2.378285	-3.254285
H	0.985620	2.906709	-3.389031
H	-0.839501	3.000300	-2.998711
H	-0.487401	-1.530175	-2.165176

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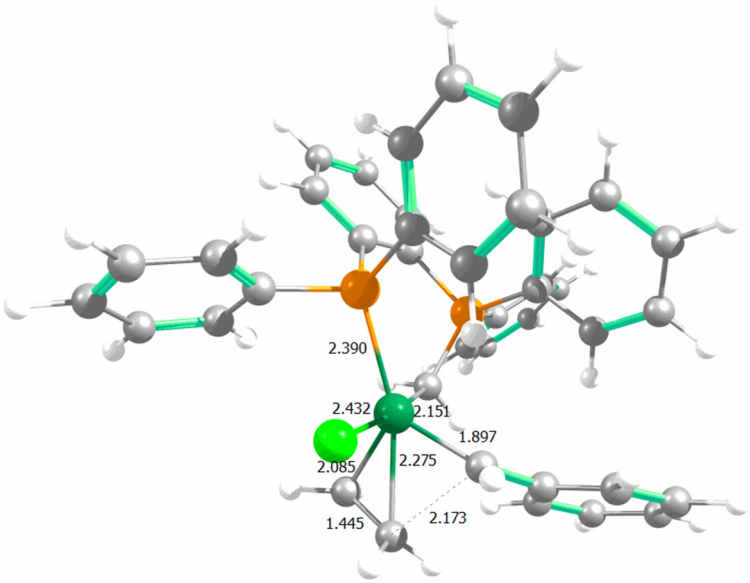


Zero-point correction = 0.622087 (Hartree/Particle)

Thermal correction to Energy = 0.662969

Thermal correction to Enthalpy = 0.663914

Thermal correction to Gibbs Free Energy = 0.547713

Sum of electronic and zero-point Energies = −2781.835609

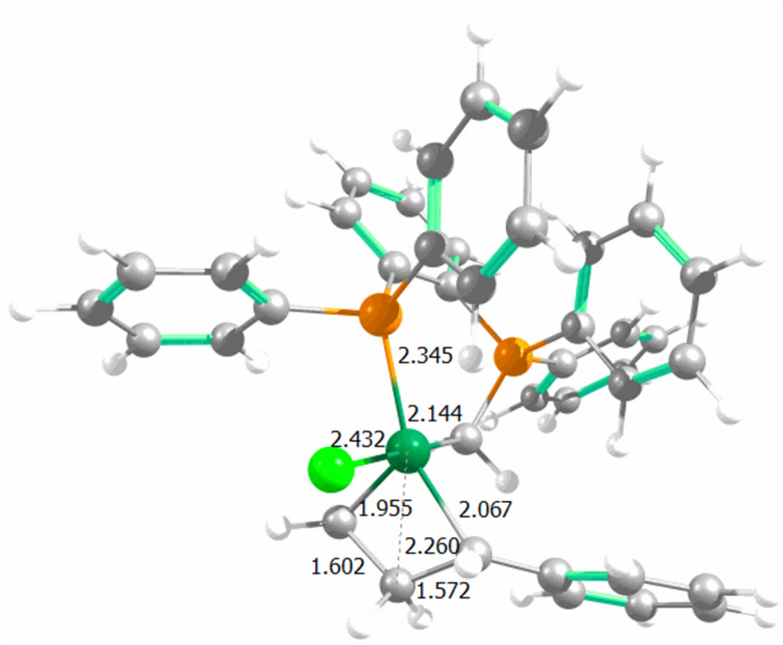
Sum of electronic and thermal Energies = −2781.794726

Sum of electronic and thermal Enthalpies = −2781.793782

Sum of electronic and thermal Free Energies = −2781.909983

P	-1.824284	0.365103	0.053973
P	1.396685	1.211882	-0.343080
C	0.897776	-0.000364	-1.583672
C	0.093294	2.490333	-0.256144
C	0.459998	3.850987	-0.347099
C	-0.521258	4.854942	-0.338589
C	-1.878374	4.504219	-0.254376
C	-2.251529	3.153339	-0.164726
C	-1.277952	2.128479	-0.143404
C	0.566433	-2.691406	-0.471495
C	-1.996706	0.132815	1.869593
C	-2.471678	1.183925	2.686434
C	-2.556906	1.007573	4.076821
C	-2.168681	-0.213732	4.658334
C	-1.702224	-1.261187	3.845458
C	-1.614332	-1.092753	2.454644
C	-3.498581	0.395811	-0.688743
C	-4.642340	0.011005	0.037494
C	-5.888460	-0.032502	-0.609715
C	-5.991683	0.290369	-1.974661
C	-4.846270	0.666090	-2.701021
C	-3.598291	0.718957	-2.061789
C	2.948029	2.051061	-0.822798
C	3.234436	2.249600	-2.192928
C	4.410625	2.916635	-2.571131
C	5.301994	3.387847	-1.589811
C	5.018202	3.192208	-0.226290
C	3.844377	2.525311	0.161757
C	1.669166	0.584180	1.342589
C	0.969868	1.137802	2.437226
C	1.220899	0.668885	3.736201
C	2.180611	-0.335499	3.947697
C	2.902673	-0.862156	2.860702
C	2.655607	-0.403408	1.558006
H	1.843262	-0.493077	-1.882921
H	1.521567	4.126852	-0.437912
H	-0.221941	5.911809	-0.410111
H	-2.655090	5.284571	-0.259823
H	-3.318516	2.886304	-0.113668
H	0.005507	-3.405966	0.177138
H	-2.766871	2.147957	2.244878
H	-2.929783	1.828822	4.708476
H	-2.233810	-0.348572	5.749380
H	-1.402189	-2.219804	4.295823
H	-1.259080	-1.917517	1.820671
H	-4.557346	-0.264298	1.099512
H	-6.784579	-0.330414	-0.043761
H	-6.970464	0.246983	-2.477066
H	-4.926036	0.918115	-3.769889
H	-2.700502	1.018400	-2.629125
H	2.542985	1.883894	-2.967851
H	4.633002	3.067924	-3.638755
H	6.224412	3.908701	-1.890350
H	5.716247	3.558638	0.542227
H	3.627887	2.369329	1.229989
H	0.223758	1.929519	2.281817
H	0.654930	1.089122	4.580813
H	2.376819	-0.703135	4.966960
H	3.667472	-1.636460	3.022668
H	3.240665	-0.802624	0.716316
Ru	-0.668384	-1.388615	-1.086677
C	2.015169	-2.917716	-0.412797
C	2.506839	-3.544918	0.764915
C	2.955060	-2.551334	-1.413671
C	3.881930	-3.732508	0.964954
H	1.791686	-3.863650	1.539897
C	4.328001	-2.745817	-1.216231
H	2.603152	-2.139959	-2.370735
C	4.799022	-3.320589	-0.018365
H	4.240008	-4.213142	1.888728
H	5.039530	-2.459433	-2.006093
H	5.879118	-3.470690	0.133671
Cl	-2.579964	-2.759050	-0.470118
C	-0.537487	-1.882080	-3.108425
H	0.206492	-1.352196	-3.731914
H	-1.587768	-1.784058	-3.448570
C	-0.170284	-3.124792	-2.469066
H	-0.947893	-3.883768	-2.279908
H	0.839328	-3.522465	-2.654571
H	0.584477	0.644764	-2.438817

A-MCy1



Zero-point correction = 0.622745 (Hartree/Particle)

Thermal correction to Energy = 0.664142

Thermal correction to Enthalpy = 0.665086

Thermal correction to Gibbs Free Energy = 0.546235

Sum of electronic and zero-point Energies = −2781.848145

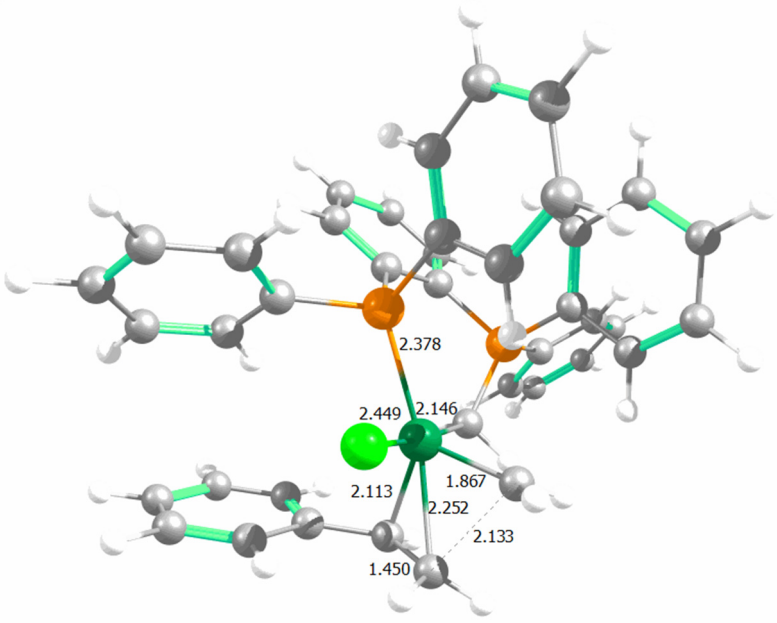
Sum of electronic and thermal Energies = −2781.806748

Sum of electronic and thermal Enthalpies = −2781.805804

Sum of electronic and thermal Free Energies = −2781.924656

P	-1.768970	0.418113	0.003286
P	1.446323	1.195738	-0.403661
C	1.063443	-0.162363	-1.513266
C	0.156253	2.480592	-0.550166
C	0.529394	3.814976	-0.819180
C	-0.448900	4.814408	-0.950024
C	-1.807184	4.484058	-0.819651
C	-2.187384	3.157872	-0.553868
C	-1.217336	2.141896	-0.400749
C	0.545072	-3.088259	-0.808055
C	-1.941212	0.378000	1.829464
C	-2.343026	1.532094	2.539365
C	-2.480607	1.480396	3.935056
C	-2.209700	0.285883	4.627879
C	-1.807074	-0.860328	3.921397
C	-1.675843	-0.822175	2.523521
C	-3.443354	0.344480	-0.735759
C	-4.560554	-0.040169	0.031521
C	-5.811992	-0.174767	-0.591901
C	-5.946068	0.057252	-1.972428
C	-4.826470	0.433262	-2.738215
C	-3.573525	0.576049	-2.124098
C	3.046473	1.988483	-0.784052
C	3.421758	2.160580	-2.136677
C	4.639268	2.785620	-2.448854
C	5.485411	3.236035	-1.418368
C	5.115709	3.060377	-0.073050
C	3.898048	2.437945	0.249458
C	1.504434	0.689572	1.339419
C	0.992645	1.524756	2.356422
C	1.070162	1.112856	3.695937
C	1.652701	-0.124943	4.020361
C	2.175583	-0.948281	3.006715
C	2.110161	-0.541435	1.666040
H	2.009459	-0.740644	-1.577551
H	1.593393	4.072987	-0.932814
H	-0.145566	5.851413	-1.160470
H	-2.580294	5.260829	-0.925564
H	-3.255259	2.905202	-0.465819
H	-0.068048	-3.752581	-0.168470
H	-2.544112	2.474967	2.008271
H	-2.802125	2.378786	4.484653
H	-2.315832	0.249678	5.723406
H	-1.597752	-1.797801	4.459105
H	-1.396497	-1.730862	1.969150
H	-4.451134	-0.243853	1.107191
H	-6.687267	-0.472386	0.005831
H	-6.928422	-0.058175	-2.456174
H	-4.930016	0.613459	-3.819484
H	-2.695880	0.868317	-2.723723
H	2.764977	1.808127	-2.947738
H	4.930410	2.919977	-3.502104
H	6.440713	3.724178	-1.666563
H	5.780037	3.408440	0.732962
H	3.612967	2.297621	1.303875
H	0.514641	2.483338	2.103083
H	0.652315	1.753477	4.486529
H	1.698209	-0.450147	5.071244
H	2.639364	-1.915356	3.253233
H	2.530504	-1.182054	0.878972
Ru	-0.610488	-1.380937	-0.956814
C	1.982500	-3.206185	-0.497809
C	2.327387	-3.729462	0.777757
C	3.038180	-2.825809	-1.366665
C	3.664964	-3.819848	1.187381
H	1.521246	-4.051903	1.456324
C	4.375811	-2.905564	-0.952756
H	2.816533	-2.479399	-2.388030
C	4.695309	-3.391493	0.329800
H	3.908184	-4.232387	2.179085
H	5.178787	-2.600568	-1.641627
H	5.746721	-3.457617	0.649407
Cl	-2.464046	-2.800255	-0.274444
C	-0.808920	-1.839601	-2.846493
H	-0.262811	-1.269203	-3.626325
H	-1.838588	-2.123764	-3.139540
C	0.025757	-3.089692	-2.291952
H	-0.645859	-3.967524	-2.370342
H	0.915899	-3.160806	-2.945170
H	0.917411	0.331612	-2.504599

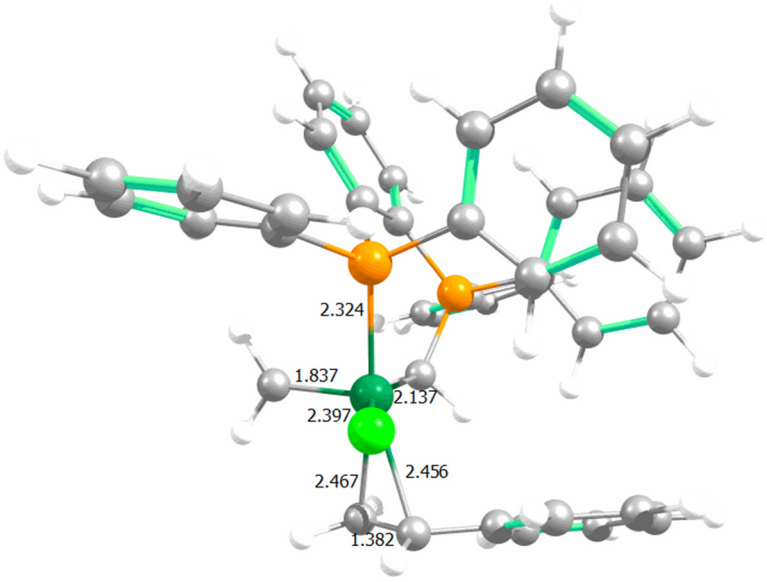
A-MCy1-CI2



Zero-point correction =	0.622213 (Hartree/Particle)
Thermal correction to Energy =	0.662763
Thermal correction to Enthalpy =	0.663707
Thermal correction to Gibbs Free Energy =	0.548106
Sum of electronic and zero-point Energies =	−2781.841997
Sum of electronic and thermal Energies =	−2781.801448
Sum of electronic and thermal Enthalpies =	−2781.800503
Sum of electronic and thermal Free Energies =	−2781.916104

P	0.762812	0.827136	0.515918
P	-2.124140	-0.822386	0.081067
C	-0.848957	-1.634981	-0.899698
C	-1.465410	-0.504724	1.756689
C	-2.216024	-0.936236	2.872570
C	-1.741184	-0.723502	4.176680
C	-0.510088	-0.078724	4.371977
C	0.240703	0.357130	3.267299
C	-0.223130	0.164123	1.946361
C	-0.009041	-0.082238	-3.076312
C	0.112619	2.537016	0.300979
C	-0.175848	3.322754	1.439923
C	-0.645706	4.636558	1.284639
C	-0.835623	5.169651	-0.003488
C	-0.553726	4.385577	-1.135347
C	-0.078331	3.072605	-0.988519
C	2.446409	0.993720	1.224550
C	3.126882	2.228287	1.219513
C	4.433438	2.301752	1.729868
C	5.060028	1.152531	2.243589
C	4.383678	-0.080561	2.234328
C	3.083109	-0.167287	1.715061
C	-3.595966	-1.889038	0.277392
C	-3.418999	-3.276575	0.488144
C	-4.538435	-4.104191	0.666082
C	-5.834223	-3.555755	0.632535
C	-6.011821	-2.177159	0.421539
C	-4.897264	-1.340006	0.244645
C	-2.724800	0.753808	-0.594520
C	-2.991778	1.836956	0.270500
C	-3.523354	3.027708	-0.249042
C	-3.787539	3.140724	-1.624513
C	-3.535156	2.056223	-2.484983
C	-3.012565	0.859350	-1.971917
H	-1.379772	-2.050808	-1.789209
H	-3.177713	-1.449393	2.720493
H	-2.334896	-1.067169	5.037497
H	-0.127172	0.090951	5.390299
H	1.206865	0.857092	3.433252
H	0.376287	0.719575	-3.744007
H	-0.034552	2.914813	2.452492
H	-0.861374	5.247157	2.175304
H	-1.204413	6.200376	-0.123446
H	-0.701472	4.797679	-2.145261
H	0.156671	2.465591	-1.873143
H	2.643111	3.126624	0.809029
H	4.965315	3.265693	1.723603
H	6.082306	1.217026	2.647778
H	4.872700	-0.985689	2.624089
H	2.570006	-1.142891	1.688244
H	-2.408651	-3.713881	0.518748
H	-4.398989	-5.183938	0.829755
H	-6.710300	-4.208444	0.769906
H	-7.025201	-1.747858	0.392870
H	-5.040724	-0.260979	0.079087
H	-2.769197	1.760084	1.345499
H	-3.713272	3.876184	0.424693
H	-4.194446	4.079764	-2.030382
H	-3.753706	2.140273	-3.560680
H	-2.843595	0.004799	-2.644133
Ru	0.862337	-0.473343	-1.472032
Cl	2.584446	1.154771	-2.087867
C	1.480615	-2.392809	-2.103966
H	0.737612	-3.208587	-2.034698
C	1.461813	-1.607428	-3.322432
H	2.370683	-1.107019	-3.694940
H	0.777988	-1.973647	-4.108434
H	-0.570885	-2.506543	-0.261646
H	-0.943404	-0.571115	-3.433653
C	2.638844	-2.560651	-1.194387
C	2.473938	-3.426043	-0.077400
C	3.892735	-1.921755	-1.379300
C	3.533535	-3.667998	0.807135
H	1.506361	-3.931986	0.073279
C	4.947635	-2.166112	-0.491524
H	4.033156	-1.217098	-2.210835
C	4.777458	-3.044503	0.595222
H	3.394726	-4.354723	1.656468
H	5.913840	-1.663453	-0.648721
H	5.616784	-3.242893	1.279969

A-CI2



Zero-point correction = 0.623330 (Hartree/Particle)

Thermal correction to Energy = 0.664525

Thermal correction to Enthalpy = 0.665469

Thermal correction to Gibbs Free Energy = 0.550365

Sum of electronic and zero-point Energies = −2781.858334

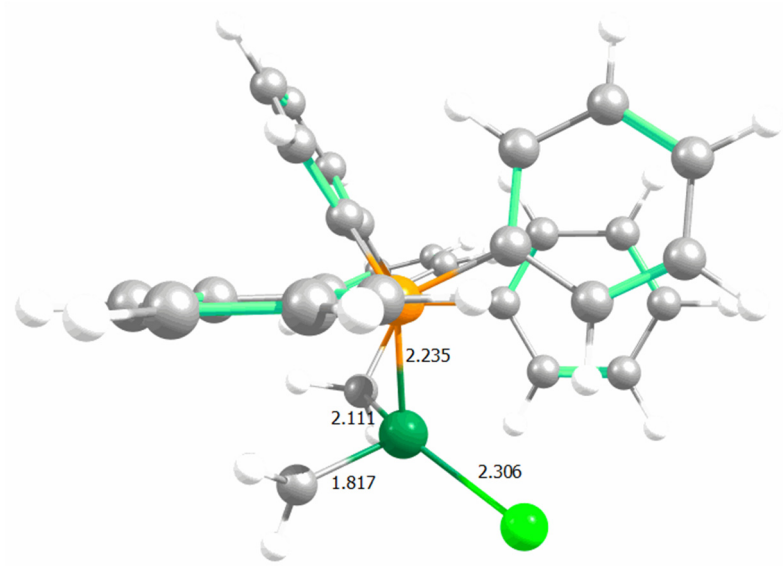
Sum of electronic and thermal Energies = −2781.817139

Sum of electronic and thermal Enthalpies = −2781.816195

Sum of electronic and thermal Free Energies = −2781.931300

P	1.680950	-0.539069	-0.046040
P	-1.643710	-1.103200	-0.313417
C	-1.212744	0.153828	-1.522864
C	-0.440141	-2.479642	-0.240929
C	-0.957396	-3.794572	-0.209829
C	-0.106101	-4.898115	-0.041783
C	1.271200	-4.689652	0.117204
C	1.793303	-3.384990	0.096020
C	0.961069	-2.258475	-0.088102
C	-0.083000	3.192696	-2.241943
C	1.534771	-0.107567	1.746415
C	1.977732	-1.031536	2.719201
C	1.916723	-0.702755	4.082186
C	1.408661	0.546008	4.483412
C	0.956395	1.460920	3.517798
C	1.018994	1.139481	2.152323
C	3.493473	-0.786984	-0.282536
C	4.391214	-0.047197	0.519353
C	5.772910	-0.116887	0.279382
C	6.273949	-0.914838	-0.763227
C	5.386723	-1.651567	-1.567437
C	4.003912	-1.587665	-1.332148
C	-3.271958	-1.819461	-0.729907
C	-3.472241	-2.335673	-2.032555
C	-4.720031	-2.869781	-2.387255
C	-5.771295	-2.886754	-1.450855
C	-5.573166	-2.374008	-0.157325
C	-4.325187	-1.841168	0.209797
C	-1.788567	-0.394706	1.350716
C	-1.509936	-1.196071	2.480130
C	-1.733515	-0.682146	3.765659
C	-2.242205	0.619754	3.925384
C	-2.512064	1.416489	2.800025
C	-2.284088	0.917094	1.508483
H	-1.947268	0.971551	-1.351953
H	-2.040209	-3.958860	-0.314645
H	-0.525099	-5.915811	-0.027666
H	1.950196	-5.543807	0.264669
H	2.875398	-3.242418	0.230755
H	0.857461	3.765765	-2.195770
H	2.383256	-2.008887	2.415458
H	2.273221	-1.423910	4.834114
H	1.363461	0.804635	5.552852
H	0.547972	2.435586	3.825599
H	0.669588	1.867599	1.406729
H	4.009777	0.593759	1.326842
H	6.461846	0.464223	0.911613
H	7.358017	-0.964874	-0.949347
H	5.771120	-2.283763	-2.382864
H	3.330340	-2.189632	-1.961940
H	-2.651452	-2.336944	-2.768387
H	-4.873836	-3.274047	-3.399652
H	-6.750670	-3.303291	-1.733151
H	-6.395039	-2.388225	0.575031
H	-4.173813	-1.442169	1.224653
H	-1.103770	-2.211764	2.355626
H	-1.499205	-1.297725	4.646950
H	-2.416030	1.019566	4.936383
H	-2.894644	2.440873	2.919129
H	-2.493333	1.558960	0.639524
Ru	0.750120	0.998200	-1.519370
C	-1.086943	3.546847	-1.211001
C	-0.647953	4.054616	0.038949
C	-2.481375	3.430001	-1.442776
C	-1.573818	4.433100	1.023420
H	0.434544	4.145424	0.221106
C	-3.404865	3.813593	-0.457958
H	-2.845587	3.080854	-2.421377
C	-2.954201	4.319340	0.777486
H	-1.214740	4.832673	1.984679
H	-4.484350	3.739889	-0.662472
H	-3.682322	4.637727	1.540034
Cl	2.473752	2.438663	-0.684078
C	1.424805	0.017667	-2.918634
H	1.355320	0.374397	-3.968604
H	1.993496	-0.929927	-2.812075
C	-0.272065	2.344299	-3.316102
H	0.471236	2.330624	-4.127939
H	-1.243446	1.875554	-3.540081
H	-1.454958	-0.288769	-2.509417

A-14e2



Zero-point correction = 0.489402 (Hartree/Particle)

Thermal correction to Energy = 0.523323

Thermal correction to Enthalpy = 0.524267

Thermal correction to Gibbs Free Energy = 0.423296

Sum of electronic and zero-point Energies = −2472.522042

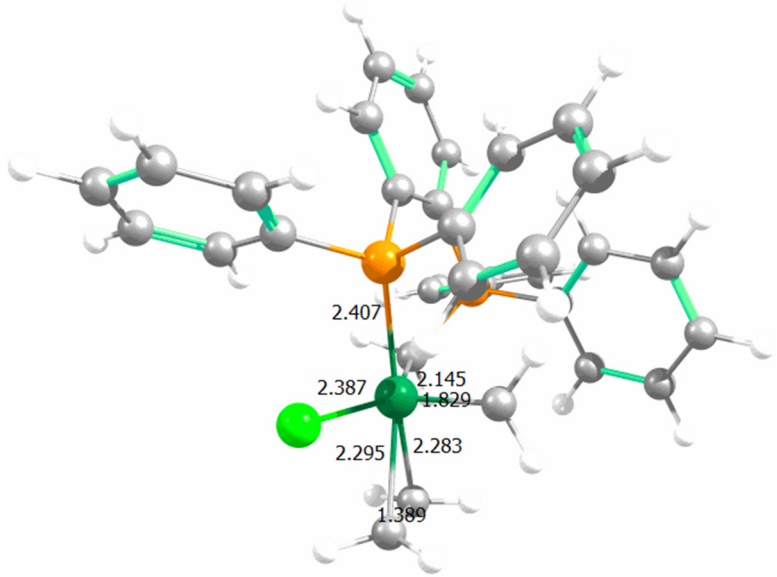
Sum of electronic and thermal Energies = −2472.488121

Sum of electronic and thermal Enthalpies = −2472.487177

Sum of electronic and thermal Free Energies = −2472.588148

P	1.334612	-0.419920	0.090011
P	-1.994056	-0.365466	-0.297833
C	-1.231975	-0.786786	-1.872775
C	-1.213889	-1.421457	0.974459
C	-2.049509	-2.173807	1.828582
C	-1.495602	-3.032559	2.792166
C	-0.101684	-3.146959	2.902011
C	0.736295	-2.393487	2.061477
C	0.203201	-1.513443	1.094022
C	1.551222	1.040491	1.216164
C	1.440517	0.885737	2.618337
C	1.671214	1.978919	3.468068
C	2.018717	3.232710	2.933004
C	2.130333	3.387831	1.541721
C	1.894929	2.300311	0.682723
C	2.960036	-1.281015	0.141645
C	4.137504	-0.538650	0.374597
C	5.390232	-1.171852	0.303560
C	5.475829	-2.541184	-0.000903
C	4.303461	-3.284036	-0.236825
C	3.048687	-2.658503	-0.172980
C	-3.788000	-0.665906	-0.267688
C	-4.291321	-1.843750	-0.868180
C	-5.669997	-2.103419	-0.837693
C	-6.544992	-1.194002	-0.213878
C	-6.044339	-0.021007	0.378420
C	-4.665928	0.249552	0.353684
C	-1.683393	1.377582	0.091178
C	-1.552289	1.787136	1.438162
C	-1.289696	3.132708	1.728591
C	-1.136823	4.062890	0.683411
C	-1.268200	3.657205	-0.655146
C	-1.557092	2.317015	-0.958247
H	-1.838405	-0.377220	-2.712928
H	-3.143438	-2.095664	1.734678
H	-2.158087	-3.614097	3.451253
H	0.343305	-3.818795	3.652318
H	1.827587	-2.479540	2.172941
H	1.170632	-0.084701	3.059380
H	1.582944	1.846911	4.557827
H	2.202068	4.087276	3.602953
H	2.398500	4.365111	1.111321
H	1.969781	2.441112	-0.405738
H	4.080075	0.533999	0.615406
H	6.304962	-0.587999	0.488961
H	6.459083	-3.033591	-0.055604
H	4.366860	-4.357432	-0.474022
H	2.135884	-3.247251	-0.359563
H	-3.610432	-2.558700	-1.357337
H	-6.064406	-3.018321	-1.305929
H	-7.626455	-1.399968	-0.194377
H	-6.730851	0.692117	0.860091
H	-4.276773	1.172662	0.810975
H	-1.625748	1.050314	2.253241
H	-1.168642	3.450705	2.774604
H	-0.904825	5.113400	0.916570
H	-1.138800	4.380909	-1.473601
H	-1.677739	2.018660	-2.011339
Ru	0.690892	0.076180	-1.992039
Cl	1.563566	2.067372	-2.762392
C	1.554732	-1.296529	-2.810866
H	1.265026	-1.465719	-3.878492
H	2.415731	-1.887313	-2.433783
H	-1.239098	-1.893734	-1.936880

A-CI3



Zero-point correction = 0.542695 (Hartree/Particle)

Thermal correction to Energy = 0.579710

Thermal correction to Enthalpy = 0.580655

Thermal correction to Gibbs Free Energy = 0.472825

Sum of electronic and zero-point Energies = −2551.020713

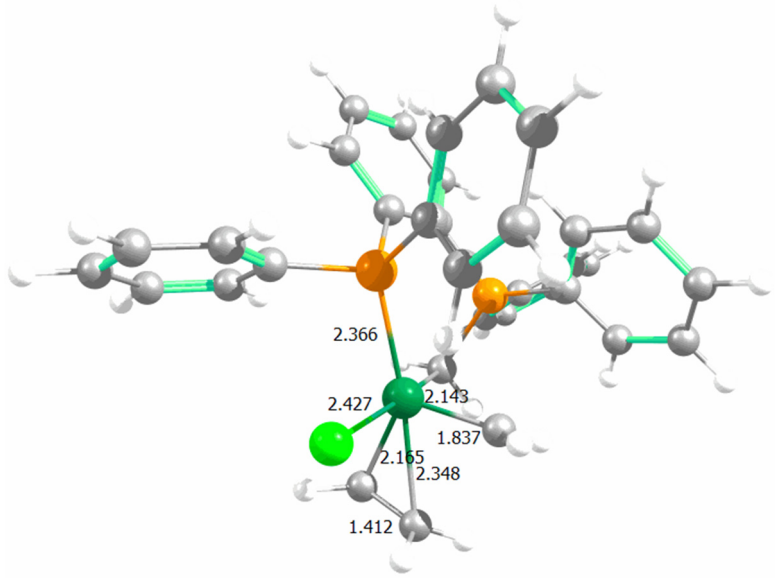
Sum of electronic and thermal Energies = −2550.983698

Sum of electronic and thermal Enthalpies = −2550.982753

Sum of electronic and thermal Free Energies = −2551.090583

P	-1.389755	0.360475	0.209444
P	2.043246	0.344739	-0.085490
C	1.190312	0.378707	-1.677036
C	1.178980	1.407744	1.111872
C	1.970679	2.223389	1.954882
C	1.367385	3.101825	2.865913
C	-0.033458	3.183201	2.926876
C	-0.822586	2.378373	2.090650
C	-0.239405	1.463022	1.182996
C	-0.246826	-2.242083	-0.989457
C	-1.937363	-0.864826	1.480933
C	-1.523527	-0.816648	2.830131
C	-1.949868	-1.803860	3.736012
C	-2.797939	-2.839250	3.307412
C	-3.223250	-2.884350	1.967162
C	-2.793508	-1.908593	1.053822
C	-2.804480	1.516785	-0.015764
C	-4.034430	1.356876	0.649820
C	-5.066376	2.288799	0.436137
C	-4.872746	3.374057	-0.434864
C	-3.641753	3.532573	-1.099676
C	-2.610625	2.605267	-0.893770
C	3.737473	0.988333	-0.270886
C	3.943139	2.142834	-1.061938
C	5.234628	2.674209	-1.196313
C	6.321180	2.059678	-0.545783
C	6.117452	0.913337	0.242346
C	4.827594	0.374045	0.385070
C	2.171614	-1.340658	0.569770
C	1.693170	-1.649516	1.858826
C	1.724548	-2.979642	2.310743
C	2.246944	-3.991692	1.487345
C	2.746647	-3.678331	0.208162
C	2.707394	-2.355814	-0.257436
H	1.968408	0.074727	-2.405709
H	3.068337	2.179795	1.885467
H	1.993654	3.730289	3.517361
H	-0.519709	3.877489	3.629556
H	-1.919099	2.452370	2.148828
H	-0.366400	-2.423093	0.099097
H	-0.873444	-0.004620	3.188621
H	-1.622057	-1.755575	4.786378
H	-3.132277	-3.609648	4.019658
H	-3.894254	-3.687731	1.625468
H	-3.124501	-1.949026	0.003500
H	-4.194220	0.504406	1.327438
H	-6.030210	2.159965	0.952713
H	-5.685087	4.098303	-0.601749
H	-3.489486	4.378454	-1.787840
H	-1.651838	2.723491	-1.426480
H	3.097724	2.631810	-1.571419
H	5.394534	3.571526	-1.813654
H	7.333859	2.477660	-0.655813
H	6.967873	0.432922	0.750209
H	4.670908	-0.523573	1.002992
H	1.277466	-0.861106	2.502524
H	1.330851	-3.222904	3.309241
H	2.268191	-5.033337	1.843308
H	3.160834	-4.471328	-0.433269
H	3.083726	-2.116188	-1.264722
Ru	-0.668816	-0.678336	-1.839232
Cl	-3.012011	-0.595933	-2.288151
C	0.472614	-1.397916	-3.681369
H	1.281800	-2.069085	-3.345581
H	0.805888	-0.503287	-4.235840
C	-0.837168	-1.843703	-3.808582
H	-1.562723	-1.299295	-4.432533
H	-1.131794	-2.873088	-3.547415
H	0.949531	1.449380	-1.878068
H	0.074554	-3.137298	-1.570829

A-CI3-MCy2



Zero-point correction = 0.541659 (Hartree/Particle)

Thermal correction to Energy = 0.578247

Thermal correction to Enthalpy = 0.579191

Thermal correction to Gibbs Free Energy = 0.471668

Sum of electronic and zero-point Energies = −2551.004417

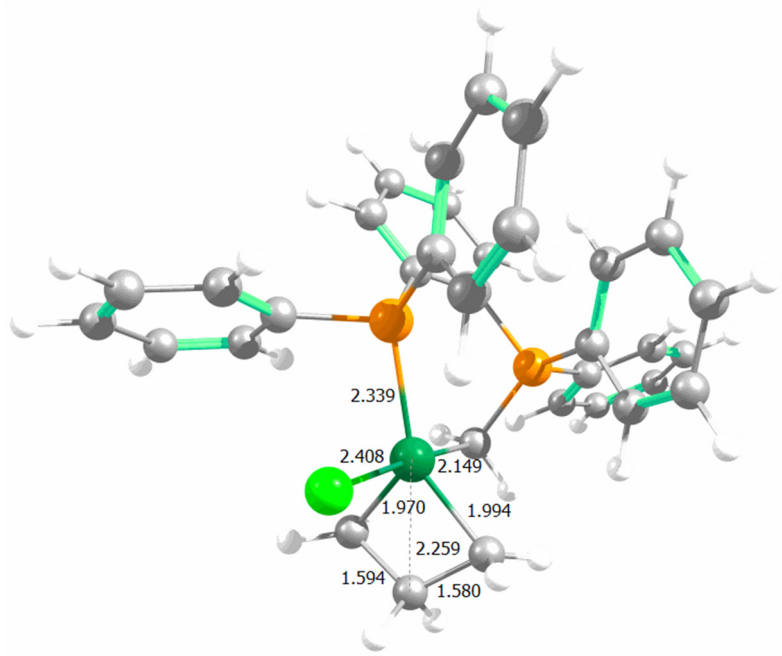
Sum of electronic and thermal Energies = −2550.967829

Sum of electronic and thermal Enthalpies = −2550.966885

Sum of electronic and thermal Free Energies = −2551.074408

P	1.348456	-0.169761	0.502378
P	-2.047869	-0.360558	-0.040148
C	-1.149922	-1.134262	-1.400984
C	-1.269247	-0.852813	1.544294
C	-2.117637	-1.319964	2.574588
C	-1.587768	-1.766584	3.794931
C	-0.198253	-1.766446	3.993411
C	0.653224	-1.306145	2.976764
C	0.139809	-0.826096	1.749468
C	0.054122	1.078749	-2.553109
C	1.738513	1.538189	1.075736
C	1.550807	1.919397	2.424234
C	1.811886	3.240945	2.822204
C	2.267335	4.185917	1.884723
C	2.474896	3.801419	0.548624
C	2.211186	2.483705	0.139829
C	2.822033	-1.220112	0.789838
C	4.091976	-0.657411	1.022708
C	5.212802	-1.498833	1.119829
C	5.071643	-2.890147	0.971855
C	3.803304	-3.450242	0.730516
C	2.677090	-2.618484	0.636039
C	-3.793089	-0.896031	0.026007
C	-4.134058	-2.202486	-0.392559
C	-5.468147	-2.634101	-0.318296
C	-6.463616	-1.769291	0.171936
C	-6.126656	-0.468885	0.588958
C	-4.795128	-0.027916	0.518218
C	-2.080514	1.455346	-0.153277
C	-1.445966	2.258792	0.813914
C	-1.410776	3.654218	0.653012
C	-2.032217	4.249252	-0.457400
C	-2.710279	3.451622	-1.400452
C	-2.739154	2.056778	-1.252156
H	-1.809754	-1.020255	-2.293492
H	-3.205998	-1.348060	2.415808
H	-2.264981	-2.126641	4.584437
H	0.229213	-2.126547	4.941996
H	1.742902	-1.318867	3.134343
H	0.697572	1.974068	-2.716465
H	1.182044	1.198360	3.169239
H	1.658622	3.532064	3.873076
H	2.468511	5.221732	2.200058
H	2.847553	4.531137	-0.186891
H	2.398340	2.176962	-0.900688
H	4.206526	0.432759	1.118495
H	6.205847	-1.061524	1.305885
H	5.955355	-3.542963	1.043546
H	3.691456	-4.539485	0.614843
H	1.681843	-3.058035	0.453104
H	-3.362626	-2.886271	-0.779805
H	-5.731819	-3.650802	-0.648054
H	-7.509250	-2.110034	0.226067
H	-6.905991	0.209308	0.969524
H	-4.536470	0.992289	0.842235
H	-0.974865	1.804644	1.695878
H	-0.887397	4.269116	1.401006
H	-2.003041	5.342476	-0.585087
H	-3.220836	3.920356	-2.255858
H	-3.281104	1.437981	-1.985882
Ru	0.826659	-0.404485	-1.793553
Cl	3.140898	0.147487	-2.270801
C	0.726682	-1.855018	-3.398035
H	-0.146930	-2.527942	-3.358154
H	1.718413	-2.328860	-3.266146
C	0.665795	-0.645145	-4.123840
H	1.585915	-0.169624	-4.499783
H	-0.283498	-0.350867	-4.603201
H	-1.133142	-2.218490	-1.141334
H	-0.993544	1.179317	-2.911351

A-MCy2



Zero-point correction = 0.544354 (Hartree/Particle)

Thermal correction to Energy = 0.580630

Thermal correction to Enthalpy = 0.581574

Thermal correction to Gibbs Free Energy = 0.475330

Sum of electronic and zero-point Energies = −2551.019436

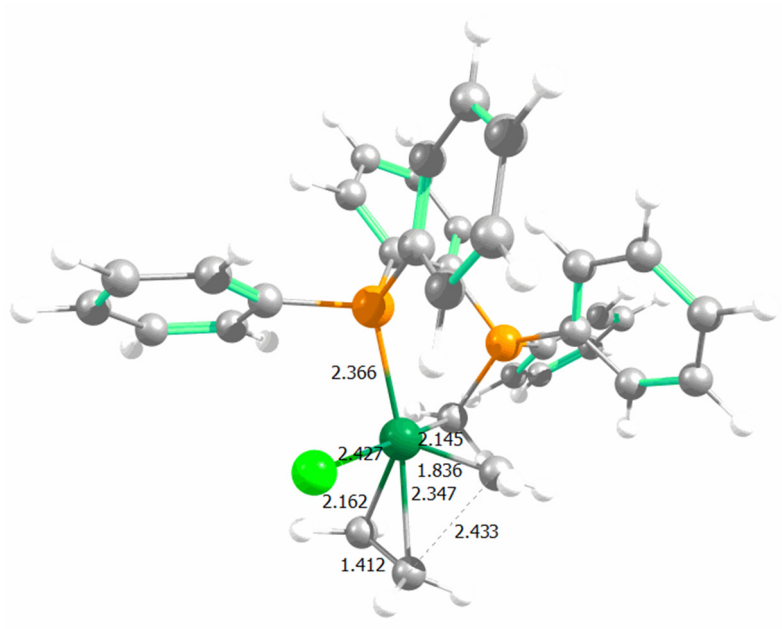
Sum of electronic and thermal Energies = −2550.983160

Sum of electronic and thermal Enthalpies = −2550.982215

Sum of electronic and thermal Free Energies = −2551.088460

P	1.212119	0.044553	0.585496
P	-2.014265	-0.423813	0.011775
C	-1.083114	-1.665738	-0.900219
C	-1.375563	-0.431822	1.724487
C	-2.260085	-0.623672	2.806116
C	-1.768975	-0.678320	4.121542
C	-0.390976	-0.552745	4.360833
C	0.496446	-0.360765	3.288101
C	0.018207	-0.280485	1.961410
C	0.172384	-0.929340	-3.313300
C	1.430538	1.866668	0.550129
C	1.288379	2.628709	1.732940
C	1.458707	4.020904	1.691272
C	1.761623	4.660387	0.474874
C	1.899594	3.902750	-0.700304
C	1.736840	2.507478	-0.670139
C	2.763748	-0.733375	1.162885
C	3.985743	-0.031803	1.106787
C	5.175548	-0.694358	1.446489
C	5.151400	-2.050473	1.821001
C	3.932278	-2.751899	1.865264
C	2.735614	-2.097796	1.535297
C	-3.802827	-0.768280	0.089347
C	-4.232962	-2.111340	0.199794
C	-5.604473	-2.399230	0.277797
C	-6.547379	-1.354947	0.242439
C	-6.120418	-0.019803	0.129105
C	-4.749856	0.279537	0.052803
C	-1.805777	1.272402	-0.614599
C	-1.727167	2.350587	0.295050
C	-1.567855	3.659179	-0.186824
C	-1.484588	3.895717	-1.569224
C	-1.583573	2.825532	-2.477355
C	-1.751425	1.515586	-2.004409
H	-1.701687	-1.938535	-1.787333
H	-3.338643	-0.739480	2.618324
H	-2.467318	-0.828300	4.959098
H	0.000390	-0.603617	5.388665
H	1.576935	-0.273296	3.481627
H	0.715308	-0.196009	-3.939442
H	1.038862	2.143938	2.688766
H	1.354726	4.609701	2.615949
H	1.892241	5.753488	0.445856
H	2.139262	4.397227	-1.654212
H	1.872541	1.915031	-1.587655
H	4.006717	1.021700	0.790125
H	6.130874	-0.148627	1.410321
H	6.090030	-2.565268	2.078563
H	3.913689	-3.813264	2.157431
H	1.779369	-2.644997	1.568563
H	-3.499333	-2.932743	0.224715
H	-5.939472	-3.444526	0.362483
H	-7.622740	-1.584679	0.299345
H	-6.858963	0.795963	0.095998
H	-4.418631	1.325570	-0.042221
H	-1.764084	2.167297	1.379958
H	-1.483195	4.493638	0.524829
H	-1.340838	4.921219	-1.942755
H	-1.529026	3.010883	-3.561011
H	-1.841688	0.685623	-2.718055
Ru	0.896472	-1.045626	-1.459595
Cl	3.054046	-0.308397	-2.235272
C	1.228934	-2.944493	-1.864311
H	0.538296	-3.731953	-1.501543
H	2.299206	-3.220332	-1.797182
C	0.841768	-2.360155	-3.296163
H	1.749652	-2.340967	-3.928531
H	0.054572	-3.046688	-3.669692
H	-1.085867	-2.552420	-0.223182
H	-0.916959	-0.963949	-3.508540

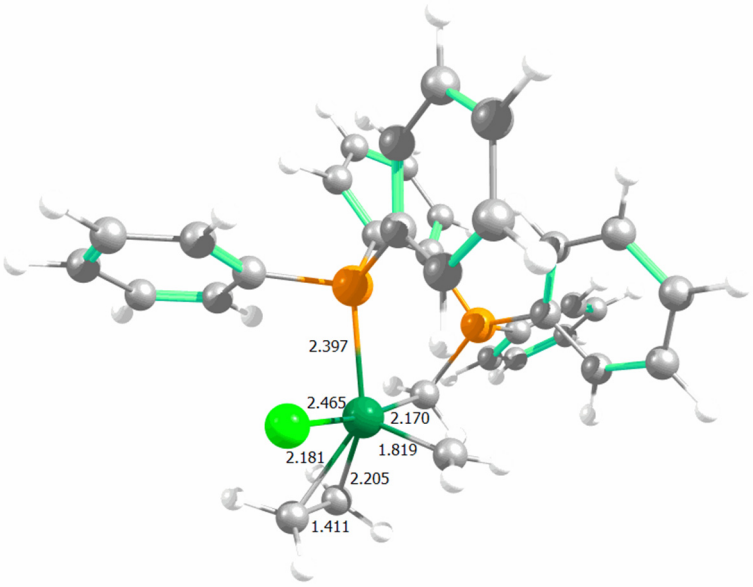
A-MCy2-CI4



Zero-point correction =	0.541592 (Hartree/Particle)
Thermal correction to Energy =	0.578187
Thermal correction to Enthalpy =	0.579131
Thermal correction to Gibbs Free Energy =	0.471706
Sum of electronic and zero-point Energies =	−2551.004447
Sum of electronic and thermal Energies =	−2550.967853
Sum of electronic and thermal Enthalpies =	−2550.966908
Sum of electronic and thermal Free Energies =	−2551.074333

P	1.336577	-0.141838	0.516493
P	-2.042849	-0.369963	-0.038705
C	-1.135677	-1.207389	-1.357228
C	-1.278791	-0.804815	1.569085
C	-2.131250	-1.244162	2.607988
C	-1.605802	-1.650016	3.844495
C	-0.217406	-1.637183	4.050349
C	0.637918	-1.204236	3.024918
C	0.128633	-0.763730	1.781182
C	0.046763	0.938156	-2.627370
C	1.714314	1.587450	1.029775
C	1.573699	1.996266	2.375790
C	1.823920	3.331485	2.732578
C	2.220306	4.262908	1.755216
C	2.376736	3.852282	0.420005
C	2.123764	2.520332	0.052921
C	2.813537	-1.176322	0.838268
C	4.082969	-0.601512	1.042994
C	5.207161	-1.435609	1.160750
C	5.069941	-2.831662	1.059817
C	3.802134	-3.404087	0.846449
C	2.672134	-2.579736	0.732969
C	-3.792928	-0.886250	0.038700
C	-4.149469	-2.200245	-0.340872
C	-5.488193	-2.614257	-0.249293
C	-6.471936	-1.724511	0.219547
C	-6.119242	-0.416032	0.596758
C	-4.783320	0.007551	0.508132
C	-2.061410	1.441058	-0.219766
C	-1.446006	2.276829	0.732725
C	-1.405451	3.665988	0.524616
C	-2.001033	4.223134	-0.618796
C	-2.661800	3.394388	-1.547223
C	-2.697928	2.005763	-1.350652
H	-1.787189	-1.138489	-2.260151
H	-3.218568	-1.282841	2.444151
H	-2.285544	-1.988900	4.641161
H	0.206287	-1.966436	5.011752
H	1.726814	-1.209185	3.188458
H	0.675162	1.832720	-2.843617
H	1.250394	1.285610	3.151134
H	1.708950	3.644257	3.782079
H	2.413982	5.309369	2.038452
H	2.700120	4.572409	-0.347501
H	2.268326	2.193678	-0.987653
H	4.193478	0.491833	1.099582
H	6.200048	-0.989284	1.324878
H	5.956589	-3.478659	1.146519
H	3.693510	-4.496968	0.767890
H	1.676909	-3.027892	0.571989
H	-3.386802	-2.903096	-0.711082
H	-5.764765	-3.636948	-0.548532
H	-7.520992	-2.051947	0.287820
H	-6.889551	0.281679	0.960046
H	-4.511323	1.033647	0.801283
H	-0.993921	1.853910	1.639959
H	-0.896587	4.305593	1.261697
H	-1.966231	5.311188	-0.783766
H	-3.154459	3.834038	-2.428173
H	-3.230203	1.363742	-2.071343
Ru	0.839579	-0.480360	-1.772216
Cl	3.142118	0.120263	-2.249369
C	0.773605	-2.039302	-3.268671
H	-0.100034	-2.710775	-3.208701
H	1.760626	-2.499643	-3.067117
C	0.738940	-0.885699	-4.082084
H	1.670908	-0.435174	-4.459679
H	-0.194575	-0.624485	-4.609183
H	-1.119704	-2.277055	-1.043395
H	-0.998091	0.991451	-3.003460

A-CI4



Zero-point correction = 0.541989 (Hartree/Particle)

Thermal correction to Energy = 0.579131

Thermal correction to Enthalpy = 0.580075

Thermal correction to Gibbs Free Energy = 0.470997

Sum of electronic and zero-point Energies = −2551.009366

Sum of electronic and thermal Energies = −2550.972225

Sum of electronic and thermal Enthalpies = −2550.971280

Sum of electronic and thermal Free Energies = −2551.080359

P	1.308022	0.034096	0.451925
P	-2.020355	-0.404365	0.002649
C	-1.102174	-1.494006	-1.112937
C	-1.267951	-0.511246	1.660907
C	-2.103223	-0.774999	2.769566
C	-1.556988	-0.927652	4.053127
C	-0.167861	-0.835240	4.233887
C	0.668582	-0.575352	3.136608
C	0.137813	-0.387153	1.838816
C	0.179351	0.280736	-2.801622
C	1.554776	1.848889	0.602383
C	1.673006	2.440413	1.881203
C	1.824083	3.831723	1.998516
C	1.860540	4.637646	0.845873
C	1.747532	4.048148	-0.425183
C	1.592130	2.658964	-0.550123
C	2.828401	-0.829791	0.996554
C	4.053534	-0.152735	1.154812
C	5.207692	-0.883901	1.479487
C	5.147045	-2.281948	1.625545
C	3.924703	-2.958026	1.458138
C	2.762241	-2.234749	1.146795
C	-3.759997	-0.940658	0.153309
C	-4.085080	-2.311489	0.036705
C	-5.416483	-2.728215	0.194904
C	-6.423380	-1.785667	0.472020
C	-6.101192	-0.421647	0.591117
C	-4.772992	0.005729	0.432295
C	-2.077548	1.344010	-0.493060
C	-1.615345	2.357289	0.371398
C	-1.691394	3.702857	-0.027175
C	-2.236064	4.037742	-1.277314
C	-2.727279	3.028730	-2.129136
C	-2.658151	1.683859	-1.738265
H	-1.754935	-1.594921	-2.008454
H	-3.189682	-0.874642	2.625384
H	-2.219050	-1.132473	4.908254
H	0.272829	-0.969275	5.233920
H	1.757626	-0.525324	3.289107
H	0.849401	0.979265	-3.349847
H	1.639983	1.825164	2.792518
H	1.916303	4.286715	2.996933
H	1.980101	5.728314	0.940783
H	1.778369	4.672630	-1.331116
H	1.510366	2.199947	-1.543973
H	4.106363	0.936855	1.011659
H	6.165617	-0.356891	1.608444
H	6.058633	-2.848535	1.870927
H	3.875317	-4.051750	1.574550
H	1.799509	-2.763645	1.037857
H	-3.304744	-3.057378	-0.179017
H	-5.668938	-3.795478	0.099165
H	-7.466530	-2.116642	0.593123
H	-6.889432	0.316376	0.805524
H	-4.524465	1.074749	0.522094
H	-1.188431	2.106595	1.353435
H	-1.311923	4.486432	0.645417
H	-2.291198	5.092212	-1.589274
H	-3.174987	3.293007	-3.099505
H	-3.074821	0.902357	-2.394213
Ru	0.918502	-0.959411	-1.694534
Cl	3.121275	0.076148	-2.084869
C	0.540923	-2.847112	-2.769835
H	-0.274805	-2.730950	-3.502659
H	0.387160	-3.656053	-2.033494
C	1.841029	-2.384389	-3.064050
H	2.718319	-2.785517	-2.526751
H	2.079347	-1.880975	-4.014229
H	-1.130163	-2.473495	-0.583708
H	-0.903553	0.342378	-3.040810

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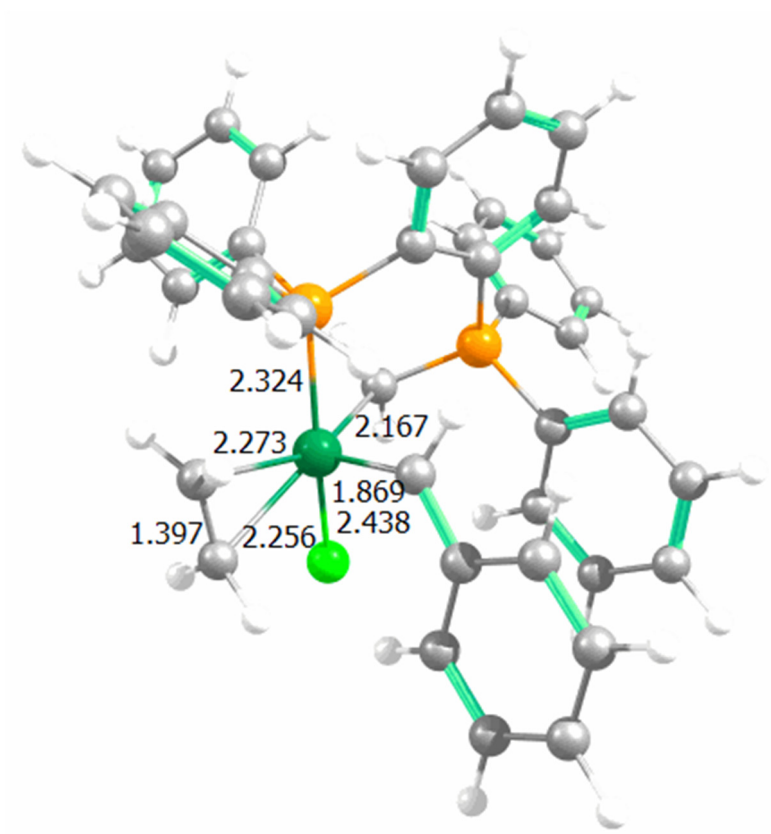

Zero-point correction = 0.622658 (Hartree/Particle)

Thermal correction to Energy = 0.664249

Thermal correction to Enthalpy = 0.665193

Thermal correction to Gibbs Free Energy = 0.546739

Sum of electronic and zero-point Energies = −2781.867658

Sum of electronic and thermal Energies = −2781.826067

Sum of electronic and thermal Enthalpies = −2781.825123

Sum of electronic and thermal Free Energies = −2781.943577

P	1.763318	0.485801	0.116199
P	-0.876115	-1.793078	0.126465
C	-0.189794	-1.081456	-1.354986
C	0.236483	-1.530903	1.555308
C	0.014457	-2.372535	2.670022
C	0.764780	-2.223624	3.846000
C	1.755297	-1.231794	3.909124
C	1.999210	-0.408188	2.797095
C	1.252925	-0.536989	1.603059
C	-0.984038	1.554774	0.074377
C	2.763792	1.810865	0.914401
C	2.094511	2.761880	1.721252
C	2.811805	3.808858	2.317646
C	4.199380	3.924797	2.104549
C	4.864739	2.988036	1.296879
C	4.152148	1.929331	0.702732
C	3.006938	-0.608978	-0.702045
C	3.302086	-0.371787	-2.064372
C	4.239544	-1.172150	-2.737025
C	4.885304	-2.220696	-2.057237
C	4.592917	-2.464082	-0.703474
C	3.658194	-1.662664	-0.024531
C	-1.064799	-3.597793	-0.031123
C	0.103035	-4.374648	-0.217434
C	-0.009885	-5.758949	-0.410526
C	-1.279834	-6.368427	-0.420124
C	-2.438528	-5.594925	-0.233626
C	-2.337548	-4.206219	-0.038346
C	-2.499953	-1.060678	0.500334
C	-2.927464	-0.866264	1.832921
C	-4.177862	-0.280609	2.082301
C	-4.998913	0.116875	1.011631
C	-4.573548	-0.080991	-0.313020
C	-3.328937	-0.673419	-0.577107
H	-0.898134	-1.315136	-2.176710
H	-0.749313	-3.164474	2.608531
H	0.577946	-2.885769	4.705215
H	2.355565	-1.102218	4.822995
H	2.797022	0.346709	2.856297
H	-0.702891	1.211420	1.099053
H	1.006569	2.685046	1.881279
H	2.285526	4.543171	2.947134
H	4.760568	4.750620	2.568557
H	5.948963	3.076255	1.126351
H	4.683174	1.195442	0.077196
H	2.793934	0.439899	-2.610552
H	4.461980	-0.978428	-3.797709
H	5.617041	-2.851399	-2.585521
H	5.097292	-3.283806	-0.168273
H	3.439791	-1.861172	1.035685
H	1.097972	-3.898174	-0.207368
H	0.896127	-6.367310	-0.555794
H	-1.364614	-7.455403	-0.573995
H	-3.429990	-6.073374	-0.240218
H	-3.244200	-3.598216	0.106826
H	-2.280849	-1.144936	2.678305
H	-4.505312	-0.118233	3.120585
H	-5.968628	0.597496	1.211811
H	-5.202651	0.247142	-1.153910
H	-2.988254	-0.766931	-1.619205
Ru	0.083493	1.068321	-1.380648
C	-2.198285	2.361547	0.143353
C	-2.670289	2.677817	1.452342
C	-2.945428	2.838671	-0.970842
C	-3.819558	3.454461	1.641493
H	-2.116875	2.295950	2.325977
C	-4.101691	3.601961	-0.775853
H	-2.625541	2.560423	-1.985593
C	-4.539749	3.919124	0.525550
H	-4.161065	3.693242	2.660643
H	-4.671383	3.956175	-1.649081
H	-5.446252	4.528039	0.669429
Cl	-1.498575	0.830179	-3.220690
C	0.229225	3.058775	-2.432382
H	-0.663261	3.645357	-2.161576
H	0.338855	2.842200	-3.507321
C	1.318526	2.967927	-1.562241
H	2.324700	2.705473	-1.936298
H	1.320171	3.502166	-0.600385
H	0.754890	-1.628849	-1.568519

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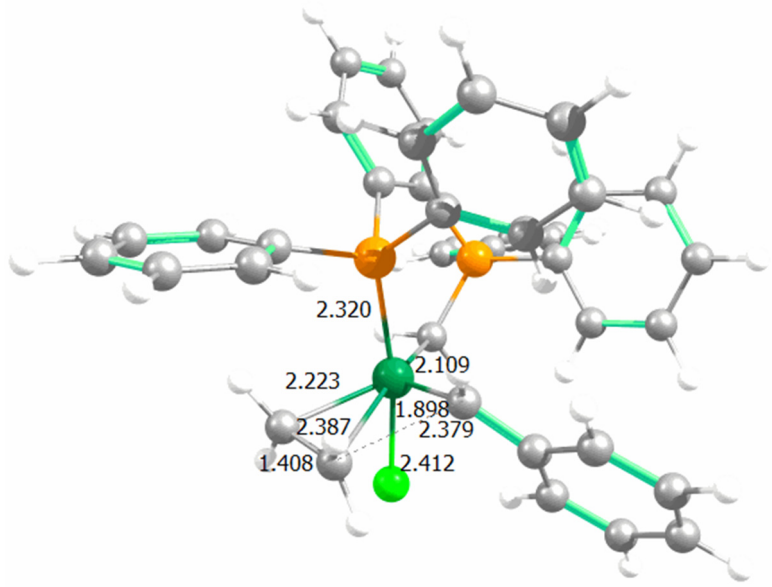

Zero-point correction = 0.623110 (Hartree/Particle)

Thermal correction to Energy = 0.663613

Thermal correction to Enthalpy = 0.664557

Thermal correction to Gibbs Free Energy = 0.550518

Sum of electronic and zero-point Energies = −2781.854457

Sum of electronic and thermal Energies = −2781.813954

Sum of electronic and thermal Enthalpies = −2781.813010

Sum of electronic and thermal Free Energies = −2781.927049

P	1.416484	-0.891495	0.167097
P	-2.013496	-0.865917	-0.235572
C	-1.158969	-0.200504	-1.653083
C	-1.120814	-2.300219	0.457429
C	-1.907456	-3.379878	0.925919
C	-1.308009	-4.508260	1.502749
C	0.089813	-4.564682	1.615395
C	0.875168	-3.495036	1.159148
C	0.297515	-2.344294	0.574992
C	1.218967	2.002257	-0.433781
C	1.614736	-0.263688	1.919527
C	0.854417	0.832883	2.378229
C	0.959474	1.270138	3.709721
C	1.813127	0.608702	4.606928
C	2.556627	-0.501715	4.166755
C	2.457842	-0.937037	2.835830
C	3.040862	-1.697483	-0.187723
C	4.235666	-1.037086	0.178741
C	5.476423	-1.516136	-0.274883
C	5.537164	-2.652093	-1.101391
C	4.350511	-3.306715	-1.479330
C	3.107422	-2.829487	-1.032358
C	-3.687165	-1.436288	-0.688110
C	-3.817493	-2.349911	-1.760711
C	-5.091333	-2.783863	-2.155324
C	-6.236568	-2.307497	-1.488757
C	-6.107833	-1.398327	-0.424852
C	-4.835233	-0.959469	-0.019478
C	-2.199041	0.410276	1.039667
C	-2.348060	0.049503	2.396042
C	-2.497151	1.054086	3.365170
C	-2.479536	2.409527	2.986380
C	-2.328772	2.766675	1.633917
C	-2.203657	1.768115	0.655239
H	-1.824371	0.546339	-2.136645
H	-3.003011	-3.338116	0.828220
H	-1.933984	-5.339913	1.860478
H	0.576763	-5.443007	2.066756
H	1.967711	-3.556978	1.267782
H	1.968953	1.880058	0.375088
H	0.163824	1.353521	1.701772
H	0.360429	2.133053	4.038486
H	1.898871	0.953440	5.649229
H	3.223259	-1.032986	4.863852
H	3.053563	-1.803708	2.512356
H	4.199228	-0.142500	0.820474
H	6.401621	-0.996764	0.019483
H	6.510295	-3.025519	-1.455757
H	4.391736	-4.192106	-2.132596
H	2.183215	-3.336723	-1.352428
H	-2.925647	-2.728666	-2.285559
H	-5.192161	-3.494315	-2.990202
H	-7.235444	-2.647024	-1.803898
H	-7.003359	-1.024297	0.094845
H	-4.739172	-0.245900	0.813324
H	-2.323226	-1.009873	2.696550
H	-2.604980	0.777280	4.424937
H	-2.578203	3.194117	3.752781
H	-2.292982	3.824253	1.330366
H	-2.079608	2.057380	-0.397514
Ru	0.817488	0.531325	-1.564830
C	0.604844	3.326950	-0.360684
C	0.943877	4.108509	0.784303
C	-0.338728	3.856567	-1.284046
C	0.353530	5.358776	1.004884
H	1.671769	3.710158	1.510028
C	-0.915165	5.113589	-1.064800
H	-0.593590	3.268559	-2.179527
C	-0.578816	5.865626	0.079323
H	0.625201	5.945908	1.895837
H	-1.634997	5.515441	-1.794757
H	-1.040599	6.851584	0.246465
Cl	0.132868	1.558129	-3.637309
C	2.936372	1.535889	-2.012647
H	3.617936	1.612708	-1.149598
H	2.717204	2.467514	-2.559321
C	2.752121	0.285600	-2.632535
H	2.424058	0.262772	-3.684915
H	3.317036	-0.588700	-2.279760
H	-1.040468	-1.036261	-2.383480

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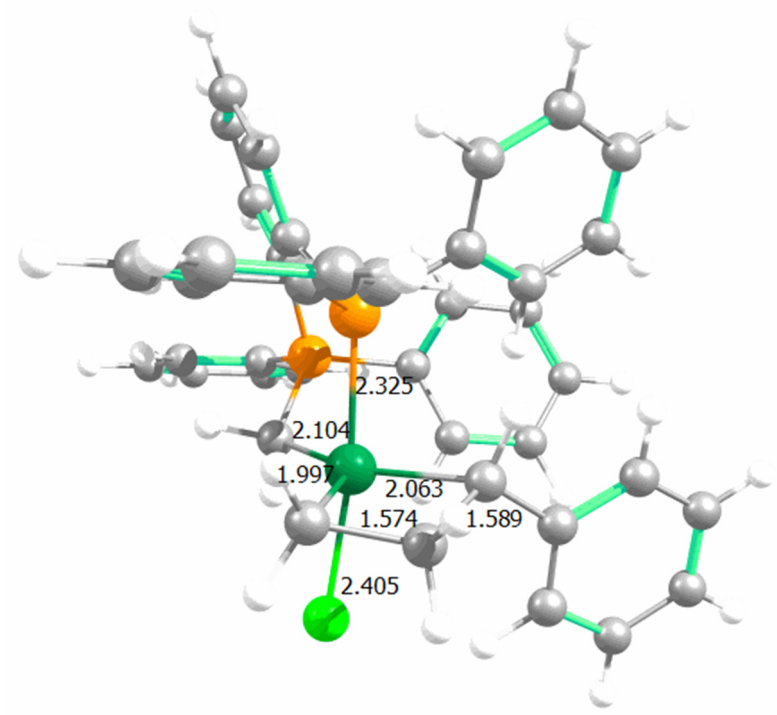

Zero-point correction = 0.624908 (Hartree/Particle)

Thermal correction to Energy = 0.665317

Thermal correction to Enthalpy = 0.666261

Thermal correction to Gibbs Free Energy = 0.552657

Sum of electronic and zero-point Energies = −2781.865908

Sum of electronic and thermal Energies = −2781.825500

Sum of electronic and thermal Enthalpies = −2781.824556

Sum of electronic and thermal Free Energies = −2781.938160

P	0.885666	-1.368496	0.128456
P	-2.276857	-0.155902	-0.196810
C	-1.336769	-0.090685	-1.711435
C	-1.940586	-1.742712	0.635561
C	-3.025870	-2.418593	1.240421
C	-2.845009	-3.683726	1.818211
C	-1.577943	-4.287175	1.779154
C	-0.493393	-3.613002	1.196030
C	-0.643039	-2.328506	0.627619
C	2.279577	1.230764	-0.611577
C	1.383402	-0.875366	1.859357
C	1.099482	0.426401	2.317160
C	1.371083	0.789825	3.647230
C	1.925928	-0.145265	4.535728
C	2.209363	-1.449336	4.087769
C	1.937603	-1.815189	2.760085
C	2.109384	-2.671747	-0.318394
C	3.475323	-2.471747	-0.013482
C	4.452551	-3.328288	-0.549758
C	4.078215	-4.386502	-1.396570
C	2.721350	-4.583198	-1.712864
C	1.741748	-3.725819	-1.185551
C	-4.063325	-0.078540	-0.540807
C	-4.620930	-1.047267	-1.409295
C	-5.984055	-0.988696	-1.732414
C	-6.792433	0.032747	-1.197422
C	-6.237589	0.997154	-0.338952
C	-4.872151	0.948137	-0.007920
C	-1.830488	1.259290	0.844422
C	-2.126146	1.227284	2.224757
C	-1.760614	2.314016	3.034195
C	-1.092192	3.418206	2.472109
C	-0.799258	3.448541	1.096965
C	-1.177744	2.376012	0.272012
H	-1.774626	0.697021	-2.360821
H	-4.025771	-1.958020	1.239801
H	-3.696962	-4.199872	2.286377
H	-1.425703	-5.286899	2.214720
H	0.495400	-4.094902	1.195615
H	2.686118	0.703686	0.272164
H	0.677582	1.170358	1.629156
H	1.147103	1.815150	3.979670
H	2.142182	0.139318	5.577302
H	2.647675	-2.187907	4.776968
H	2.170638	-2.837569	2.425759
H	3.779940	-1.645508	0.648944
H	5.513302	-3.167907	-0.301395
H	4.845112	-5.056618	-1.814713
H	2.423528	-5.405860	-2.381387
H	0.684586	-3.873206	-1.459844
H	-3.993874	-1.850150	-1.829761
H	-6.418246	-1.741521	-2.408157
H	-7.861771	0.077511	-1.455931
H	-6.868939	1.798029	0.075509
H	-4.440935	1.710401	0.659340
H	-2.615030	0.345717	2.669549
H	-1.979404	2.288502	4.112636
H	-0.788632	4.260521	3.112916
H	-0.258828	4.301021	0.658731
H	-0.935135	2.415682	-0.803871
Ru	0.735094	0.234523	-1.548160
C	2.281979	2.691128	-0.332861
C	2.668011	3.097741	0.972644
C	1.925634	3.696417	-1.267134
C	2.682029	4.451557	1.338777
H	2.970632	2.335384	1.707644
C	1.948688	5.049965	-0.901846
H	1.599360	3.405546	-2.276515
C	2.318670	5.435701	0.402100
H	2.989559	4.740042	2.356115
H	1.668963	5.814437	-1.643492
H	2.329613	6.500496	0.683142
Cl	0.313624	1.703307	-3.405839
C	2.942122	0.655722	-1.936387
H	3.887928	0.213574	-1.557290
H	3.115024	1.480551	-2.651877
C	2.209214	-0.539845	-2.650420
H	2.076190	-0.357174	-3.733184
H	2.611522	-1.540459	-2.416670
H	-1.436928	-1.071070	-2.226833

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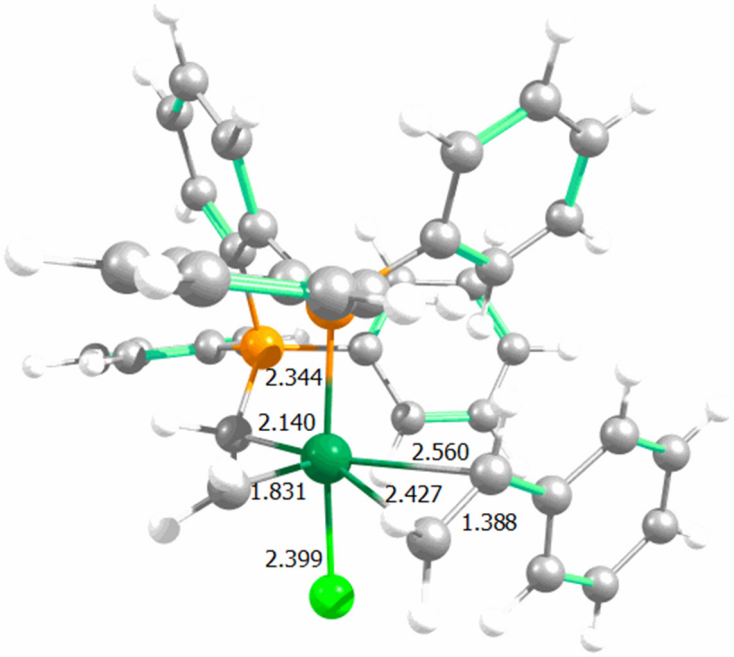


Zero-point correction = 0.622968 (Hartree/Particle)

Thermal correction to Energy = 0.663543

Thermal correction to Enthalpy = 0.664487

Thermal correction to Gibbs Free Energy = 0.550196

Sum of electronic and zero-point Energies = −2781.852142

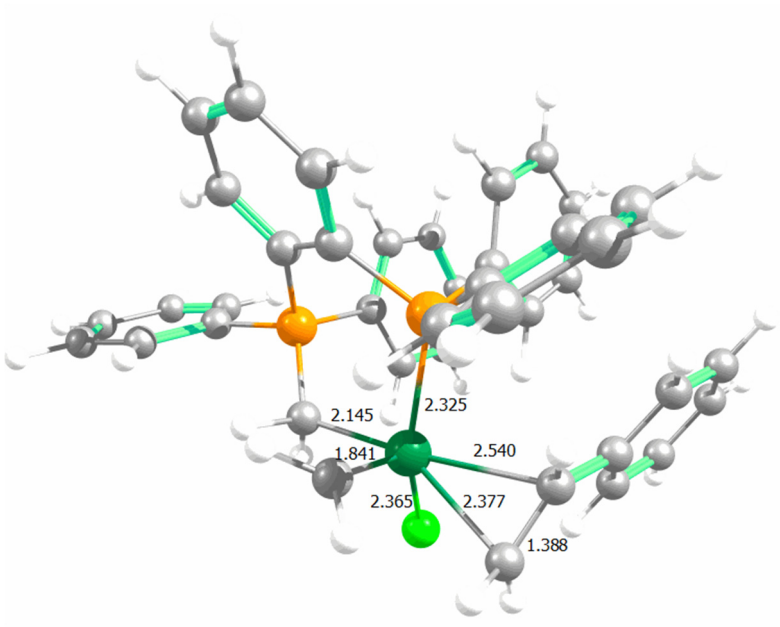
Sum of electronic and thermal Energies = −2781.811567

Sum of electronic and thermal Enthalpies = −2781.810623

Sum of electronic and thermal Free Energies = −2781.924914

P	0.823919	-1.392177	0.172990
P	-2.321296	-0.014103	-0.219343
C	-1.509490	-0.131919	-1.804652
C	-2.030366	-1.555270	0.729314
C	-3.142057	-2.133802	1.385952
C	-3.007607	-3.324215	2.115603
C	-1.754957	-3.952444	2.191907
C	-0.644250	-3.378193	1.554740
C	-0.750765	-2.175295	0.820946
C	2.868177	1.010378	-0.848837
C	1.512643	-0.819503	1.793528
C	1.307047	0.515947	2.189113
C	1.702002	0.945287	3.467670
C	2.313302	0.047948	4.357540
C	2.532603	-1.286067	3.963618
C	2.130799	-1.722035	2.691832
C	1.880863	-2.827995	-0.294871
C	3.285307	-2.700556	-0.212298
C	4.118655	-3.690545	-0.761084
C	3.559479	-4.812014	-1.399143
C	2.161777	-4.939775	-1.490902
C	1.324371	-3.950323	-0.948902
C	-4.125521	0.192560	-0.393750
C	-4.819625	-0.687404	-1.257904
C	-6.202649	-0.539494	-1.438026
C	-6.896058	0.484748	-0.765351
C	-6.206217	1.362450	0.088462
C	-4.820495	1.221564	0.277797
C	-1.689141	1.394657	0.738529
C	-1.852430	1.408900	2.142163
C	-1.356205	2.490459	2.886020
C	-0.671566	3.537056	2.238851
C	-0.505449	3.519433	0.843262
C	-1.031074	2.461112	0.081834
H	-1.905657	0.669501	-2.464220
H	-4.128470	-1.650688	1.315969
H	-3.884262	-3.759724	2.618971
H	-1.635509	-4.889900	2.756771
H	0.332507	-3.877964	1.635748
H	3.126906	0.357339	0.003014
H	0.860809	1.236802	1.490981
H	1.537062	1.994894	3.755011
H	2.626888	0.385925	5.357512
H	3.020854	-1.993024	4.652280
H	2.310275	-2.767431	2.398203
H	3.735860	-1.829409	0.288746
H	5.211992	-3.583852	-0.686846
H	4.213869	-5.586869	-1.827343
H	1.718219	-5.814590	-1.991278
H	0.231135	-4.052160	-1.041845
H	-4.282743	-1.490104	-1.788673
H	-6.742289	-1.223691	-2.110771
H	-7.981007	0.600946	-0.912794
H	-6.747355	2.167338	0.609274
H	-4.283542	1.916540	0.941386
H	-2.344450	0.566599	2.654321
H	-1.478854	2.501055	3.979804
H	-0.256109	4.369916	2.827066
H	0.047443	4.324337	0.336632
H	-0.908089	2.476551	-1.014333
Ru	0.611487	0.089343	-1.630723
C	2.775701	2.440216	-0.481894
C	3.103096	2.809220	0.848594
C	2.458780	3.470653	-1.403674
C	3.084543	4.151070	1.255666
H	3.398151	2.029570	1.566550
C	2.438430	4.811215	-0.994934
H	2.199733	3.216105	-2.440337
C	2.743576	5.159188	0.335968
H	3.352634	4.412075	2.291472
H	2.186841	5.595427	-1.725918
H	2.730311	6.214972	0.649284
Cl	0.246835	1.816461	-3.255172
C	2.958880	0.463591	-2.121529
H	3.365582	-0.553887	-2.233947
H	2.948992	1.093477	-3.024361
C	0.873324	-1.304295	-2.789303
H	0.185593	-1.419112	-3.659081
H	1.708544	-2.037640	-2.753222
H	-1.817438	-1.115104	-2.220129

A-CI2-cis



Zero-point correction =	0.622481 (Hartree/Particle)
Thermal correction to Energy =	0.663737
Thermal correction to Enthalpy =	0.664681
Thermal correction to Gibbs Free Energy =	0.548598
Sum of electronic and zero-point Energies =	−2781.862867
Sum of electronic and thermal Energies =	−2781.821611
Sum of electronic and thermal Enthalpies =	−2781.820667
Sum of electronic and thermal Free Energies =	−2781.936750

P	0.761345	-1.086834	0.169468
P	-2.425854	-0.058534	-0.190136
C	-1.592706	-0.138003	-1.771433
C	-2.009547	-1.567081	0.758461
C	-3.051626	-2.261729	1.410625
C	-2.799266	-3.469943	2.081194
C	-1.500564	-3.998867	2.091793
C	-0.451696	-3.305691	1.462028
C	-0.680345	-2.079375	0.802204
C	3.081386	0.055422	-1.848635
C	0.937827	0.155120	1.521291
C	1.202593	1.505827	1.222758
C	1.398557	2.429060	2.260960
C	1.328641	2.011336	3.600259
C	1.034735	0.669320	3.904167
C	0.828995	-0.257064	2.870184
C	2.186667	-2.244655	0.379675
C	3.152612	-2.063933	1.391790
C	4.246419	-2.944007	1.485518
C	4.378454	-4.011547	0.582325
C	3.410127	-4.202547	-0.421791
C	2.324760	-3.320090	-0.526233
C	-4.237399	-0.066396	-0.425595
C	-4.812416	-1.083300	-1.225093
C	-6.195506	-1.091065	-1.456818
C	-7.009789	-0.087055	-0.899045
C	-6.439932	0.923760	-0.106391
C	-5.054794	0.939696	0.133720
C	-2.022306	1.442312	0.737916
C	-2.128400	1.448143	2.145628
C	-1.939534	2.649106	2.845365
C	-1.653777	3.835720	2.144367
C	-1.539270	3.822297	0.743303
C	-1.722524	2.626579	0.030193
H	-1.998295	0.705905	-2.370160
H	-4.076546	-1.861803	1.379191
H	-3.622993	-3.998646	2.584686
H	-1.292424	-4.952126	2.601977
H	0.566613	-3.719912	1.502975
H	3.395305	-0.929029	-1.462001
H	1.257483	1.853395	0.181290
H	1.607958	3.479146	2.010903
H	1.489880	2.736470	4.413105
H	0.962201	0.341140	4.952765
H	0.591808	-1.304009	3.115836
H	3.063338	-1.227817	2.099894
H	5.001280	-2.788145	2.271882
H	5.237579	-4.695987	0.657245
H	3.505122	-5.038837	-1.131546
H	1.578375	-3.467967	-1.323193
H	-4.184204	-1.876041	-1.662368
H	-6.640582	-1.882899	-2.078864
H	-8.094766	-0.093408	-1.086455
H	-7.075669	1.710425	0.328252
H	-4.613901	1.736751	0.752003
H	-2.342766	0.515886	2.691550
H	-2.007724	2.657402	3.943637
H	-1.507589	4.776101	2.698282
H	-1.300820	4.747476	0.196452
H	-1.604410	2.617280	-1.064562
Ru	0.546575	-0.089237	-1.919240
C	3.522409	1.205839	-1.033239
C	4.295370	0.959179	0.128277
C	3.212626	2.550190	-1.365156
C	4.729941	2.013985	0.944253
H	4.563913	-0.077551	0.382225
C	3.642565	3.601819	-0.544590
H	2.604781	2.769455	-2.255106
C	4.399157	3.339886	0.614988
H	5.331642	1.801011	1.841507
H	3.390160	4.639165	-0.815239
H	4.737406	4.170105	1.254618
Cl	0.110452	1.952634	-3.029101
C	2.575810	0.109454	-3.140361
H	2.585550	-0.797229	-3.764470
H	2.499068	1.058051	-3.690958
C	0.407152	-1.769943	-2.657524
H	1.162197	-2.159075	-3.379457
H	-0.469647	-2.449183	-2.526199
H	-1.991087	-1.073897	-2.226428

A-CI3-cis

Zero-point correction =	0.542699 (Hartree/Particle)
Thermal correction to Energy =	0.579560
Thermal correction to Enthalpy =	0.580504
Thermal correction to Gibbs Free Energy =	0.473004
Sum of electronic and zero-point Energies =	−2551.024710
Sum of electronic and thermal Energies =	−2550.987849
Sum of electronic and thermal Enthalpies =	−2550.986905
Sum of electronic and thermal Free Energies =	−2551.094405

P	-1.627695	0.183190	0.102178
P	1.849776	0.257131	0.145288
C	0.911089	-0.083113	-1.336605
C	0.798352	0.854082	1.520094
C	1.503487	1.418658	2.607881
C	0.823200	1.874364	3.747251
C	-0.576202	1.782494	3.797877
C	-1.286592	1.245536	2.710745
C	-0.620041	0.769354	1.559524
C	-0.146057	-2.391576	0.455536
C	-3.301296	-0.033681	0.834406
C	-3.509562	-1.104626	1.736003
C	-4.780570	-1.324343	2.286962
C	-5.856676	-0.486516	1.935391
C	-5.654520	0.574205	1.037185
C	-4.379847	0.805769	0.487516
C	-1.761427	1.725051	-0.912475
C	-2.093286	1.596562	-2.280825
C	-2.184431	2.734108	-3.099121
C	-1.936029	4.009835	-2.560489
C	-1.601585	4.144108	-1.201372
C	-1.514999	3.008096	-0.376571
C	3.050393	1.592876	-0.158065
C	2.539592	2.842718	-0.582361
C	3.424165	3.898403	-0.845014
C	4.811466	3.712964	-0.685891
C	5.316137	2.471854	-0.261491
C	4.439116	1.405690	0.006061
C	2.719173	-1.243246	0.682215
C	2.631774	-1.718108	2.010757
C	3.280238	-2.911623	2.365278
C	4.012342	-3.630478	1.402920
C	4.101170	-3.155843	0.082429
C	3.457040	-1.964782	-0.285158
H	1.626834	-0.508226	-2.070671
H	2.601042	1.505547	2.559523
H	1.387606	2.304675	4.588511
H	-1.125346	2.140658	4.682400
H	-2.384977	1.202687	2.755128
H	-0.412131	-2.084393	1.491177
H	-2.675464	-1.770917	2.010117
H	-4.934837	-2.157462	2.990132
H	-6.855422	-0.664664	2.363098
H	-6.493131	1.231584	0.759778
H	-4.229509	1.643964	-0.210199
H	-2.271281	0.600295	-2.717570
H	-2.444639	2.622776	-4.163083
H	-2.001649	4.901275	-3.203383
H	-1.407813	5.141213	-0.775939
H	-1.252852	3.126609	0.685940
H	1.452510	2.993385	-0.700200
H	3.031036	4.872222	-1.175374
H	5.502870	4.544249	-0.893925
H	6.400508	2.329238	-0.135969
H	4.835128	0.434144	0.340696
H	2.048233	-1.169579	2.765195
H	3.208094	-3.284080	3.398648
H	4.514078	-4.569558	1.683523
H	4.662426	-3.723017	-0.675338
H	3.513406	-1.620625	-1.327883
Ru	-0.629001	-1.549191	-1.096975
Cl	0.940602	-2.918571	-2.361786
C	-1.964715	-2.952318	-2.183073
H	-1.709685	-3.973865	-1.861733
H	-1.796026	-2.750589	-3.255182
C	-2.794901	-2.124714	-1.413707
H	-3.352643	-1.289455	-1.872786
H	-3.223790	-2.483134	-0.465180
H	0.519626	0.879593	-1.728096
H	0.486409	-3.299840	0.361008

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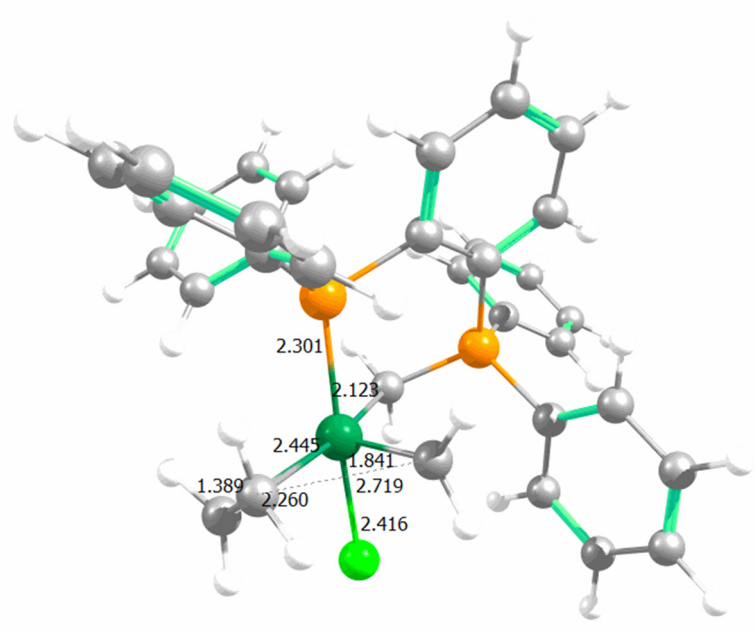


Zero-point correction = 0.541088 (Hartree/Particle)

Thermal correction to Energy = 0.577853

Thermal correction to Enthalpy = 0.578797

Thermal correction to Gibbs Free Energy = 0.470157

Sum of electronic and zero-point Energies = −2551.015855

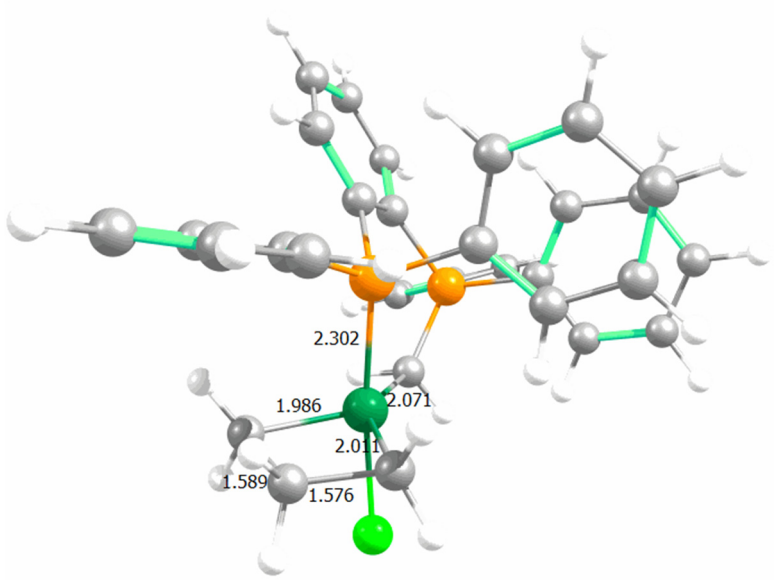
Sum of electronic and thermal Energies = −2550.979090

Sum of electronic and thermal Enthalpies = −2550.978146

Sum of electronic and thermal Free Energies = −2551.086786

P	-1.614458	-0.281571	-0.111540
P	1.871273	-0.223198	-0.124995
C	0.932365	-0.015859	1.382383
C	0.853689	-0.893315	-1.493975
C	1.590269	-1.446525	-2.568021
C	0.938248	-1.972077	-3.693398
C	-0.464434	-1.969908	-3.741971
C	-1.203656	-1.440425	-2.671224
C	-0.567866	-0.883789	-1.538665
C	-0.181914	2.413135	-0.312045
C	-3.264089	-0.044411	-0.904141
C	-3.383879	0.927984	-1.927222
C	-4.630932	1.188506	-2.513824
C	-5.774078	0.490395	-2.079001
C	-5.661563	-0.471878	-1.061861
C	-4.411416	-0.743897	-0.475281
C	-1.792457	-1.820318	0.903469
C	-2.334451	-1.687437	2.203010
C	-2.439561	-2.804365	3.047558
C	-1.988861	-4.062591	2.608007
C	-1.442100	-4.200202	1.320145
C	-1.345251	-3.086236	0.466697
C	3.218940	-1.424971	0.120312
C	2.865794	-2.730564	0.536287
C	3.871468	-3.680648	0.764255
C	5.224220	-3.334400	0.579151
C	5.572871	-2.038266	0.162635
C	4.573034	-1.077292	-0.070199
C	2.584965	1.366304	-0.646769
C	2.524014	1.799089	-1.990824
C	3.062812	3.047740	-2.342051
C	3.659605	3.860298	-1.361271
C	3.722056	3.425938	-0.024405
C	3.189528	2.180552	0.339731
H	1.630609	0.383642	2.148818
H	2.690647	-1.472313	-2.518171
H	1.527489	-2.391374	-4.523147
H	-0.991466	-2.391519	-4.611889
H	-2.302741	-1.465552	-2.712616
H	-0.480619	2.247574	-1.371109
H	-2.494943	1.480372	-2.272989
H	-4.712802	1.941367	-3.313171
H	-6.753627	0.698347	-2.536594
H	-6.552060	-1.022993	-0.721739
H	-4.334188	-1.508811	0.312399
H	-2.677417	-0.702087	2.559295
H	-2.867721	-2.689909	4.055416
H	-2.062818	-4.937141	3.272760
H	-1.091128	-5.184343	0.971984
H	-0.919575	-3.209390	-0.540859
H	1.806631	-3.005994	0.676758
H	3.600840	-4.697070	1.089341
H	6.011155	-4.082647	0.761400
H	6.630502	-1.769478	0.017402
H	4.846578	-0.062024	-0.396949
H	2.043745	1.174319	-2.759124
H	3.011276	3.388461	-3.387576
H	4.074803	4.841433	-1.639515
H	4.174342	4.066551	0.747714
H	3.205406	1.874800	1.395895
Ru	-0.644844	1.385272	1.143870
Cl	0.676524	2.760711	2.627303
C	-2.615300	2.799582	0.838385
H	-3.318890	2.201491	0.241452
H	-2.343283	3.786943	0.429280
C	-2.325042	2.500010	2.163718
H	-1.868284	3.241611	2.837131
H	-2.830711	1.640740	2.646307
H	0.584002	-1.022295	1.702057
H	0.442115	3.313842	-0.123953

A-MCy2-cis



Zero-point correction = 0.545493 (Hartree/Particle)

Thermal correction to Energy = 0.581193

Thermal correction to Enthalpy = 0.582137

Thermal correction to Gibbs Free Energy = 0.478433

Sum of electronic and zero-point Energies = −2551.037190

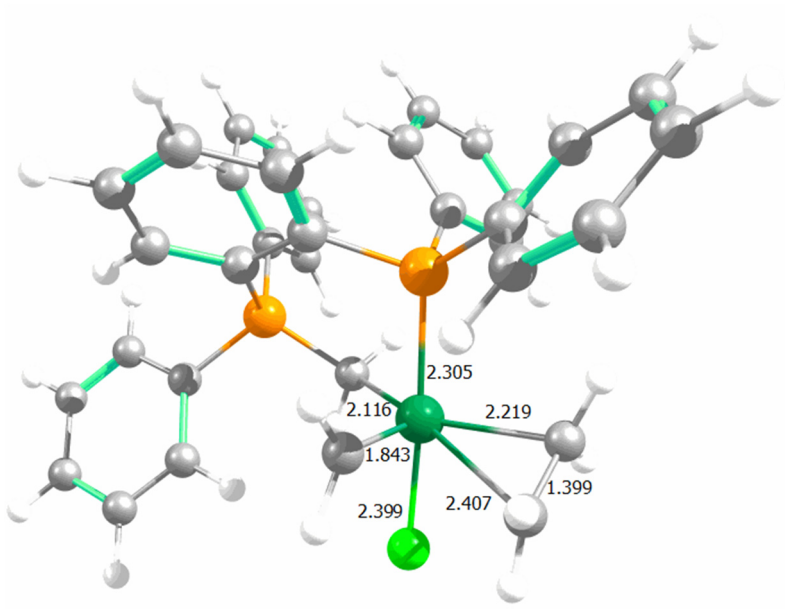
Sum of electronic and thermal Energies = −2551.001490

Sum of electronic and thermal Enthalpies = −2551.000545

Sum of electronic and thermal Free Energies = −2551.104250

P	-1.356854	-0.108179	0.406463
P	1.967472	0.327630	0.202499
C	1.091312	1.572824	-0.753532
C	1.151923	-0.009858	1.801678
C	1.981199	-0.150323	2.937721
C	1.433165	-0.485908	4.185456
C	0.050567	-0.695601	4.299687
C	-0.779437	-0.564971	3.173116
C	-0.254912	-0.219206	1.908285
C	-2.403545	0.854602	-2.296607
C	-1.208881	-1.841368	-0.248548
C	-0.908801	-2.072980	-1.606573
C	-0.828701	-3.386216	-2.099324
C	-1.041523	-4.476857	-1.239311
C	-1.326709	-4.253149	0.120241
C	-1.409539	-2.942038	0.614774
C	-3.073494	-0.076301	1.079877
C	-4.080537	-0.868220	0.481515
C	-5.426820	-0.699879	0.850361
C	-5.782759	0.252729	1.820760
C	-4.786366	1.040761	2.425457
C	-3.441082	0.885717	2.052903
C	3.659284	0.909826	0.550812
C	3.830472	2.188815	1.131705
C	5.123230	2.663218	1.398423
C	6.243738	1.869636	1.087059
C	6.073127	0.598735	0.511188
C	4.782538	0.112574	0.240592
C	2.108220	-1.219642	-0.732292
C	2.080373	-2.459148	-0.057443
C	2.283145	-3.643891	-0.781199
C	2.520367	-3.593067	-2.166679
C	2.544417	-2.357347	-2.837490
C	2.337597	-1.165458	-2.125141
H	1.652909	1.752109	-1.695979
H	3.066751	0.007220	2.845989
H	2.089643	-0.585820	5.063168
H	-0.390999	-0.968734	5.270701
H	-1.859189	-0.744740	3.282906
H	-2.859681	-0.134999	-2.105592
H	-0.719479	-1.225618	-2.282471
H	-0.590353	-3.555057	-3.160443
H	-0.980407	-5.505551	-1.627387
H	-1.491103	-5.104679	0.798896
H	-1.640839	-2.776629	1.678826
H	-3.813811	-1.628945	-0.268421
H	-6.201280	-1.324915	0.379199
H	-6.837349	0.379374	2.110367
H	-5.057629	1.784298	3.191000
H	-2.670427	1.508004	2.536278
H	2.959230	2.814634	1.384142
H	5.257605	3.658991	1.848058
H	7.257100	2.247432	1.293645
H	6.949998	-0.020536	0.267359
H	4.651384	-0.881813	-0.213151
H	1.880452	-2.499005	1.024442
H	2.246153	-4.612623	-0.260850
H	2.679028	-4.525764	-2.729776
H	2.723827	-2.318719	-3.922885
H	2.356993	-0.203317	-2.659932
Ru	-0.949230	1.575550	-1.108895
Cl	-0.406260	3.159017	-2.812115
C	-3.142219	2.039270	-1.565593
H	-4.027533	1.593618	-1.067601
H	-3.385733	2.795757	-2.337554
C	-2.350497	2.802212	-0.418398
H	-2.140701	3.858142	-0.675068
H	-2.794445	2.659649	0.582734
H	1.127279	2.529311	-0.179291
H	-2.217234	1.052750	-3.369283

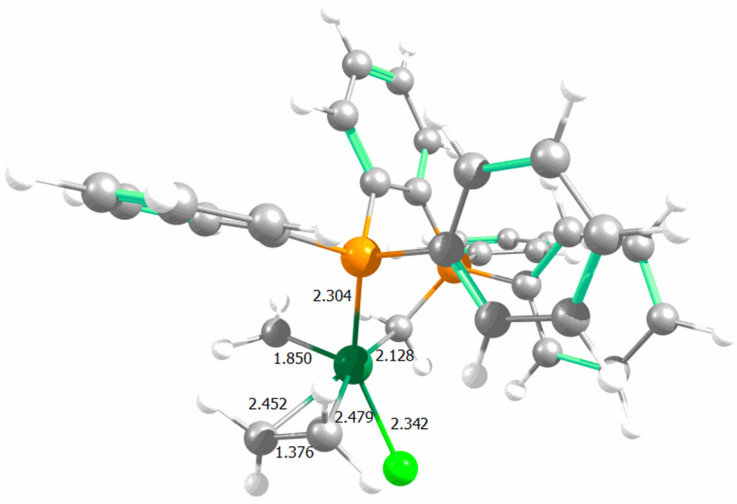
A-MCy2-CI4-cis



Zero-point correction =	0.541939 (Hartree/Particle)
Thermal correction to Energy =	0.578337
Thermal correction to Enthalpy =	0.579281
Thermal correction to Gibbs Free Energy =	0.472891
Sum of electronic and zero-point Energies =	−2551.019912
Sum of electronic and thermal Energies =	−2550.983514
Sum of electronic and thermal Enthalpies =	−2550.982570
Sum of electronic and thermal Free Energies =	−2551.088960

P	1.542660	0.238425	0.154771
P	-1.825102	-0.032270	0.082554
C	-0.901027	-0.659162	-1.333119
C	-0.876628	0.093277	1.653516
C	-1.620874	0.014374	2.850097
C	-1.000537	0.223692	4.094054
C	0.369190	0.520597	4.145480
C	1.122539	0.582508	2.958544
C	0.520704	0.366346	1.702233
C	3.014723	-1.872636	-1.734342
C	1.165410	1.800828	-0.748554
C	1.424614	1.847901	-2.137962
C	1.097477	2.994352	-2.879040
C	0.505993	4.099933	-2.239032
C	0.258472	4.062751	-0.856359
C	0.588526	2.918572	-0.110362
C	3.279281	0.443316	0.732163
C	4.020223	1.615726	0.472120
C	5.360700	1.706687	0.888638
C	5.966285	0.636014	1.568142
C	5.230627	-0.534920	1.832359
C	3.895872	-0.634846	1.411483
C	-3.216297	-1.163353	0.382533
C	-3.010505	-2.553200	0.214283
C	-4.068574	-3.438290	0.473653
C	-5.317899	-2.947601	0.897333
C	-5.520174	-1.564924	1.054950
C	-4.471888	-0.665983	0.795610
C	-2.471671	1.645470	-0.241772
C	-2.637500	2.587816	0.797632
C	-3.119571	3.873344	0.503122
C	-3.432478	4.224505	-0.821976
C	-3.273838	3.284774	-1.856100
C	-2.798539	1.995083	-1.571042
H	-0.631624	0.205047	-1.976956
H	-2.695800	-0.222080	2.813731
H	-1.591986	0.149390	5.019339
H	0.864145	0.693187	5.113738
H	2.201233	0.793745	3.013196
H	3.718948	-1.111282	-1.360399
H	1.878351	0.979120	-2.644486
H	1.300333	3.023693	-3.960829
H	0.238258	4.994470	-2.822451
H	-0.208477	4.923333	-0.353780
H	0.378887	2.891507	0.970100
H	3.552377	2.458330	-0.059804
H	5.934154	2.623025	0.679141
H	7.016199	0.710919	1.891147
H	5.701572	-1.376059	2.364506
H	3.326752	-1.554686	1.619789
H	-2.042426	-2.944813	-0.138746
H	-3.916388	-4.519606	0.334443
H	-6.143451	-3.648551	1.096216
H	-6.502128	-1.181110	1.371770
H	-4.635189	0.418568	0.900643
H	-2.372929	2.330703	1.834454
H	-3.244228	4.606874	1.314652
H	-3.803177	5.235900	-1.050191
H	-3.521588	3.555820	-2.893796
H	-2.680133	1.267286	-2.388859
Ru	0.931706	-1.661794	-0.998827
Cl	-0.021100	-3.383591	-2.371407
C	2.862224	-3.096703	-1.073843
H	3.374444	-3.268078	-0.112624
H	2.438259	-3.975658	-1.583792
C	0.864367	-2.634027	0.564961
H	0.511930	-3.687982	0.488709
H	1.122381	-2.293596	1.592998
H	-1.589987	-1.326692	-1.891872
H	2.766155	-1.836370	-2.813983

A-CI4-cis



Zero-point correction = 0.544161 (Hartree/Particle)

Thermal correction to Energy = 0.580597

Thermal correction to Enthalpy = 0.581541

Thermal correction to Gibbs Free Energy = 0.476567

Sum of electronic and zero-point Energies = −2551.027932

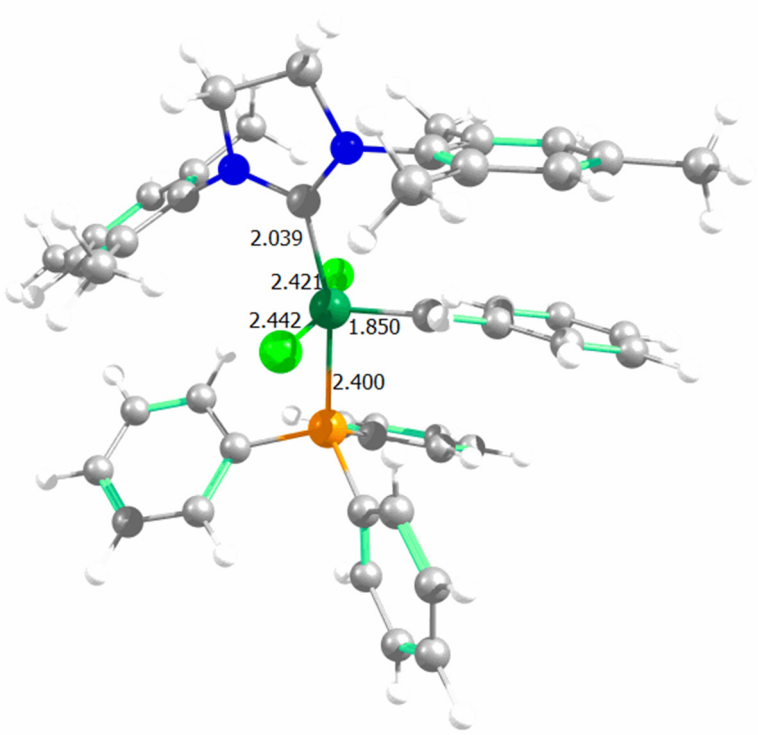
Sum of electronic and thermal Energies = −2550.991495

Sum of electronic and thermal Enthalpies = −2550.990551

Sum of electronic and thermal Free Energies = −2551.095525

15	-1.382394	-0.341284	-0.306927
15	1.963778	-0.443028	0.141724
6	1.176186	-0.751135	1.719935
6	1.132060	-1.403334	-1.183319
6	1.939403	-2.147850	-2.071929
6	1.363166	-2.916862	-3.096657
6	-0.031327	-2.952002	-3.240624
6	-0.845645	-2.205403	-2.371644
6	-0.285178	-1.416220	-1.344532
6	-2.907218	1.234967	2.104632
6	-1.307126	1.274344	-1.196623
6	-1.168799	2.482625	-0.482216
6	-1.165533	3.707811	-1.167665
6	-1.296802	3.734590	-2.566712
6	-1.415646	2.531013	-3.284944
6	-1.417399	1.302703	-2.605318
6	-3.090281	-0.966253	-0.606868
6	-4.103824	-0.123960	-1.111771
6	-5.422692	-0.601275	-1.223829
6	-5.734692	-1.917943	-0.848114
6	-4.723294	-2.765364	-0.355753
6	-3.409988	-2.290010	-0.226793
6	3.712234	-0.967759	0.162620
6	4.025044	-2.260854	0.645237
6	5.361765	-2.683549	0.691901
6	6.389363	-1.821361	0.264463
6	6.079925	-0.535622	-0.211280
6	4.743546	-0.103237	-0.264555
6	1.940896	1.320426	-0.278128
6	1.979313	1.722305	-1.631409
6	2.070575	3.086582	-1.944468
6	2.126620	4.043285	-0.913818
6	2.074066	3.640633	0.432095
6	1.978964	2.278095	0.759419
1	1.800277	-0.246654	2.490502
1	3.033804	-2.134096	-1.957396
1	2.010019	-3.491313	-3.777199
1	-0.493935	-3.555988	-4.036510
1	-1.938286	-2.230712	-2.501410
1	-3.378209	1.329062	1.112432
1	-1.040434	2.476165	0.611272
1	-1.049889	4.644830	-0.602486
1	-1.297822	4.697188	-3.101317
1	-1.510291	2.547662	-4.381840
1	-1.512356	0.365194	-3.175025
1	-3.870723	0.906907	-1.419489
1	-6.209323	0.065276	-1.609940
1	-6.767748	-2.287854	-0.937987
1	-4.960558	-3.800801	-0.066112
1	-2.625077	-2.959832	0.162034
1	3.227096	-2.943355	0.979385
1	5.603640	-3.689732	1.067462
1	7.437962	-2.154543	0.306482
1	6.883680	0.140431	-0.541212
1	4.507340	0.907031	-0.632461
1	1.923828	0.972507	-2.436201
1	2.088324	3.405288	-2.997527
1	2.199137	5.113149	-1.163988
1	2.102078	4.390238	1.237805
1	1.911546	1.974822	1.816090
44	-0.851177	-0.138014	1.926129
17	-0.085189	1.209130	3.681849
6	-3.100611	0.108506	2.870272
1	-3.710857	-0.724908	2.482665
1	-2.846768	0.095429	3.942666
6	-1.241634	-1.934787	2.133952
1	-2.195621	-2.308052	2.566289
1	-0.498717	-2.744162	1.935752
1	1.290058	-1.847852	1.882229
1	-2.485562	2.152116	2.548615

B-PPh$_3$



Zero-point correction = 0.785461 (Hartree/Particle)

Thermal correction to Energy = 0.838440

Thermal correction to Enthalpy = 0.839385

Thermal correction to Gibbs Free Energy = 0.697424

Sum of electronic and zero-point Energies = −3245.374771

Sum of electronic and thermal Energies = −3245.321791

Sum of electronic and thermal Enthalpies = −3245.320847

Sum of electronic and thermal Free Energies = −3245.462807

Ru	-0.077612	-0.325392	-0.233493
Cl	-0.620670	-0.325334	2.126068
Cl	-0.201145	-0.420644	-2.670086
P	-0.704822	1.991295	-0.260497
N	-1.140627	-3.151395	-0.376502
N	1.048285	-3.152397	-0.606764
C	-0.031412	-2.360795	-0.342849
C	-0.846697	-4.514564	-0.862092
H	-1.185967	-4.617740	-1.917113
H	-1.375565	-5.273544	-0.250875
C	0.683304	-4.579817	-0.732005
H	1.015884	-5.134890	0.175320
H	1.176362	-5.037812	-1.612570
C	-2.455714	-2.790543	0.074611
C	-2.754594	-2.988074	1.449776
C	-1.715233	-3.544954	2.390481
H	-2.150363	-3.763284	3.385085
H	-0.896165	-2.808338	2.525076
H	-1.262847	-4.480924	1.999240
C	-4.041306	-2.652980	1.902543
H	-4.280190	-2.785841	2.971087
C	-5.032873	-2.162727	1.026933
C	-6.405467	-1.807386	1.554446
H	-7.066815	-1.415446	0.755883
H	-6.342241	-1.038691	2.354859
H	-6.905967	-2.692118	2.003637
C	-4.713343	-2.026153	-0.335281
H	-5.478212	-1.653844	-1.036219
C	-3.435204	-2.342721	-0.842238
C	-3.151683	-2.257080	-2.320293
H	-3.891718	-1.610185	-2.831028
H	-3.213529	-3.265125	-2.788125
H	-2.140924	-1.849781	-2.527091
C	2.425169	-2.785194	-0.458601
C	3.219295	-2.611810	-1.618160
C	2.609845	-2.752619	-2.990417
H	3.333385	-2.475814	-3.782172
H	1.708270	-2.107752	-3.086393
H	2.281791	-3.796225	-3.189632
C	4.572444	-2.258011	-1.444623
H	5.198168	-2.102130	-2.339396
C	5.140621	-2.087693	-0.166959
C	6.581121	-1.665291	0.004694
H	7.114695	-2.324401	0.721435
H	6.632459	-0.633069	0.414510
H	7.136024	-1.679493	-0.954672
C	4.322388	-2.287796	0.962784
H	4.748188	-2.144345	1.969549
C	2.966227	-2.639381	0.845720
C	2.096934	-2.801560	2.065395
H	1.474657	-3.719017	2.014274
H	1.383983	-1.952752	2.159278
H	2.704595	-2.845063	2.989805
C	1.730634	0.046053	-0.348238
C	3.960463	1.035576	-0.023105
C	2.715727	0.650322	0.549976
C	4.966296	1.618287	0.758880
C	2.520745	0.859164	1.940420
C	4.763142	1.797396	2.141207
H	5.915590	1.928349	0.293466
C	3.541555	1.410949	2.724949
H	1.551685	0.586431	2.384230
H	5.556822	2.243979	2.761769
H	3.372291	1.563069	3.802590
C	-2.522524	2.038013	-0.580281
C	-3.087474	2.775267	-1.644034
C	-3.360773	1.239080	0.234915
C	-4.474961	2.747269	-1.863054
H	-2.442862	3.367174	-2.310711
C	-4.749749	1.242674	0.026658
H	-2.924506	0.603343	1.024503
C	-5.311029	1.995678	-1.018737
H	-4.904352	3.322015	-2.699179
H	-5.393120	0.636151	0.679621
H	-6.400339	1.987009	-1.183590
C	0.050234	3.172716	-1.464349
C	-0.266804	4.549388	-1.371249
C	0.981823	2.740505	-2.428182
C	0.333122	5.474919	-2.238607
H	-0.977176	4.896848	-0.604037
C	1.585147	3.673230	-3.291288
H	1.211139	1.669433	-2.520024
C	1.263319	5.037560	-3.200605
H	0.080256	6.544102	-2.157379
H	2.311144	3.324593	-4.042924
H	1.738824	5.764739	-3.878256
C	-0.430304	2.913053	1.319539
C	-1.400806	3.009132	2.337795
C	0.859651	3.445411	1.542365
C	-1.087064	3.637814	3.554489
H	-2.409301	2.599778	2.183451
C	1.170753	4.066183	2.762396
H	1.629622	3.370975	0.759104
C	0.198326	4.164451	3.772520
H	-1.855170	3.710406	4.340829
H	2.184731	4.465160	2.922472
H	0.441743	4.651100	4.730522
H	4.125109	0.862850	-1.098520
H	2.174821	-0.171549	-1.348850

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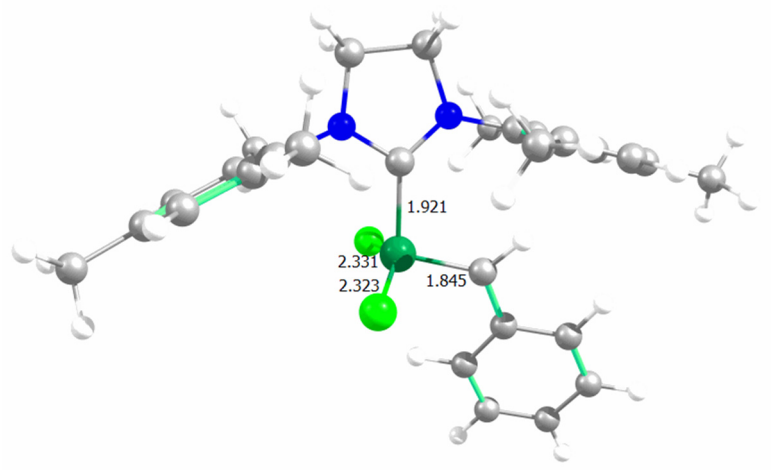
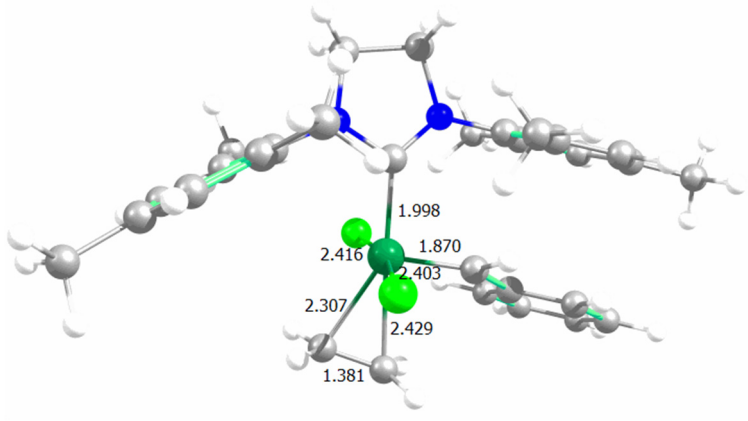


Zero-point correction =	0.516062 (Hartree/Particle)
Thermal correction to Energy =	0.552313
Thermal correction to Enthalpy =	0.553257
Thermal correction to Gibbs Free Energy =	0.443607
Sum of electronic and zero-point Energies =	−2209.811377
Sum of electronic and thermal Energies =	−2209.775126
Sum of electronic and thermal Enthalpies =	−2209.774182
Sum of electronic and thermal Free Energies =	−2209.883832

Ru	-0.263881	0.811780	-0.007758
Cl	-0.364966	1.369128	2.253292
Cl	-1.003863	1.250927	-2.165366
N	-1.881123	-1.532326	0.389179
N	0.243037	-2.133456	0.430837
C	-0.595982	-1.064019	0.237702
C	-1.932581	-2.923472	0.857696
H	-2.683608	-3.505973	0.285487
H	-2.219262	-2.959001	1.933761
C	-0.487004	-3.399713	0.621551
H	-0.067948	-3.964919	1.479147
H	-0.391689	-4.040670	-0.285332
C	-3.061023	-0.753311	0.153840
C	-3.699197	-0.072757	1.217989
C	-3.263565	-0.242554	2.653267
H	-3.320963	0.716540	3.204520
H	-2.220659	-0.599408	2.735014
H	-3.930749	-0.968158	3.169470
C	-4.820190	0.726620	0.907532
H	-5.314562	1.280854	1.722983
C	-5.323924	0.830368	-0.401110
C	-6.492266	1.734220	-0.723280
H	-7.218377	1.236427	-1.399475
H	-6.143607	2.652765	-1.244084
H	-7.032991	2.053964	0.189937
C	-4.704040	0.075924	-1.421387
H	-5.105183	0.121997	-2.447458
C	-3.582470	-0.727586	-1.167870
C	-2.941806	-1.558226	-2.252930
H	-3.470655	-1.435077	-3.217674
H	-2.950042	-2.639268	-1.993133
H	-1.885947	-1.258356	-2.403025
C	1.650651	-2.154986	0.185873
C	2.114818	-2.303481	-1.142800
C	1.139345	-2.336421	-2.295358
H	1.636447	-2.625934	-3.241413
H	0.689832	-1.327333	-2.435196
H	0.293327	-3.032141	-2.121012
C	3.506425	-2.263181	-1.363719
H	3.884772	-2.359248	-2.395128
C	4.419005	-2.063364	-0.307954
C	5.909268	-2.011041	-0.559992
H	6.409606	-2.929992	-0.183904
H	6.376209	-1.152265	-0.033738
H	6.143006	-1.921716	-1.639686
C	3.913108	-1.907470	1.000400
H	4.614729	-1.725801	1.831685
C	2.533612	-1.950776	1.273081
C	1.983042	-1.688588	2.652700
H	1.280166	-2.485998	2.974037
H	1.406148	-0.737505	2.663325
H	2.792182	-1.617475	3.405287
C	1.562010	0.850154	-0.269143
C	3.754047	1.931840	-0.609277
C	2.395445	2.043860	-0.195180
C	4.611745	3.038648	-0.570406
C	1.936353	3.306715	0.276552
C	4.135468	4.281863	-0.111896
H	5.659003	2.934682	-0.896358
C	2.797840	4.409341	0.313031
H	0.900921	3.408030	0.638519
H	4.809273	5.152887	-0.079265
H	2.427876	5.378956	0.682013
H	4.119621	0.951851	-0.959004
H	2.111775	-0.053135	-0.587283

B-CI1



Zero-point correction = 0.569460 (Hartree/Particle)

Thermal correction to Energy = 0.608231

Thermal correction to Enthalpy = 0.609175

Thermal correction to Gibbs Free Energy = 0.498335

Sum of electronic and zero-point Energies = −2288.313028

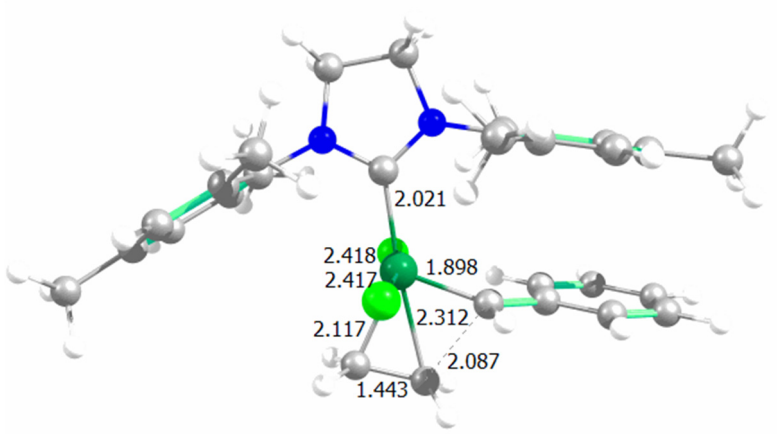
Sum of electronic and thermal Energies = −2288.274257

Sum of electronic and thermal Enthalpies = −2288.273313

Sum of electronic and thermal Free Energies = −2288.384153

Ru	-0.496927	0.903437	-0.278173
Cl	-0.247721	1.611256	2.018168
Cl	-1.184870	0.400742	-2.525457
N	-1.812589	-1.460935	0.834103
N	0.356549	-1.841137	0.813623
C	-0.610445	-0.963278	0.423759
C	-1.674819	-2.652051	1.689474
H	-2.400271	-3.436938	1.392947
H	-1.868513	-2.383717	2.752228
C	-0.207046	-3.053252	1.445410
H	0.338390	-3.296679	2.379436
H	-0.108782	-3.923621	0.756752
C	-3.074529	-0.880230	0.470332
C	-3.740172	0.011269	1.348348
C	-3.263271	0.232036	2.762210
H	-3.589106	1.217772	3.148494
H	-2.159875	0.194138	2.839888
H	-3.694006	-0.545493	3.432258
C	-4.925170	0.622660	0.886554
H	-5.441479	1.338056	1.548517
C	-5.471031	0.334577	-0.377930
C	-6.711762	1.040776	-0.875955
H	-7.420227	0.331947	-1.353290
H	-6.448357	1.799301	-1.645277
H	-7.245871	1.566016	-0.058919
C	-4.831682	-0.635474	-1.179347
H	-5.270891	-0.906936	-2.153667
C	-3.643774	-1.264945	-0.773741
C	-2.980990	-2.318849	-1.625007
H	-3.645251	-2.642126	-2.449995
H	-2.705216	-3.214508	-1.029253
H	-2.051794	-1.910408	-2.074236
C	1.730783	-1.812904	0.415189
C	2.073964	-2.263497	-0.883954
C	1.000139	-2.669551	-1.863975
H	1.431877	-3.163638	-2.755864
H	0.419580	-1.782052	-2.207577
H	0.258431	-3.359188	-1.410804
C	3.434144	-2.244133	-1.251232
H	3.716113	-2.577223	-2.264088
C	4.435894	-1.800546	-0.365635
C	5.888557	-1.755535	-0.777542
H	6.273986	-0.714699	-0.723736
H	6.039804	-2.123545	-1.811904
H	6.519740	-2.369000	-0.099880
C	4.053793	-1.369077	0.921626
H	4.825169	-0.999243	1.617192
C	2.711647	-1.369468	1.338146
C	2.307918	-0.872479	2.701694
H	1.835365	-1.677012	3.306350
H	1.557642	-0.056974	2.615842
H	3.182449	-0.494344	3.265716
C	1.296617	0.803374	-0.797480
C	3.661379	1.239983	-1.299071
C	2.546485	1.464373	-0.440102
C	4.915488	1.797319	-1.017524
C	2.742914	2.259507	0.722641
C	5.094614	2.563054	0.149283
H	5.759270	1.628778	-1.705232
C	4.006175	2.785607	1.017125
H	1.887709	2.420438	1.396849
H	6.082861	2.991560	0.381755
H	4.146238	3.384069	1.931419
C	-1.481474	2.969211	-0.572213
C	-0.181673	3.209627	-0.971805
H	-2.257521	2.712589	-1.314091
H	-1.811493	3.234050	0.446276
H	0.110872	3.127756	-2.030895
H	3.525447	0.610467	-2.192386
H	1.445937	0.095562	-1.642353
H	0.556848	3.635536	-0.274706

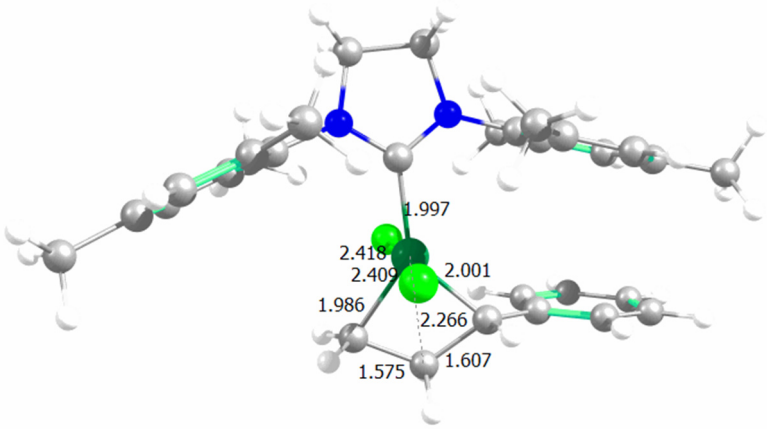
B-CI1-MCy1



Zero-point correction =	0.569723 (Hartree/Particle)
Thermal correction to Energy =	0.607470
Thermal correction to Enthalpy =	0.608414
Thermal correction to Gibbs Free Energy =	0.499438
Sum of electronic and zero-point Energies =	−2288.309166
Sum of electronic and thermal Energies =	−2288.271418
Sum of electronic and thermal Enthalpies =	−2288.270474
Sum of electronic and thermal Free Energies =	−2288.379451

Ru	0.406544	-0.900878	-0.343683
Cl	0.274353	-1.610333	1.963873
Cl	0.965580	-0.357732	-2.631258
N	1.928631	1.466421	0.729178
N	-0.238830	1.867566	0.677613
C	0.723765	0.968675	0.356388
C	1.801996	2.728986	1.485183
H	2.527307	3.481165	1.113838
H	2.010728	2.546602	2.562571
C	0.331400	3.116957	1.228851
H	-0.207446	3.415920	2.150280
H	0.226165	3.940240	0.486498
C	3.188375	0.831776	0.456523
C	3.801783	0.010615	1.434458
C	3.241128	-0.106902	2.830206
H	3.590669	-1.033090	3.326971
H	2.133987	-0.126658	2.829413
H	3.580238	0.750645	3.453726
C	5.002431	-0.640558	1.083426
H	5.481275	-1.299832	1.826604
C	5.607905	-0.464442	-0.175120
C	6.869294	-1.209401	-0.549949
H	7.600073	-0.544182	-1.055573
H	6.642126	-2.035401	-1.259041
H	7.364321	-1.657156	0.334986
C	5.008708	0.428523	-1.088330
H	5.492060	0.611576	-2.062521
C	3.808698	1.098202	-0.793108
C	3.197170	2.078688	-1.762312
H	3.897684	2.312888	-2.587339
H	2.920391	3.030939	-1.262259
H	2.272777	1.649745	-2.205890
C	-1.628429	1.780522	0.325439
C	-2.027540	2.122159	-0.991754
C	-1.014592	2.519765	-2.035416
H	-1.502241	3.001326	-2.905419
H	-0.451361	1.630424	-2.398514
H	-0.254523	3.222103	-1.634551
C	-3.399100	2.047553	-1.301105
H	-3.725331	2.298846	-2.324392
C	-4.361138	1.668680	-0.343407
C	-5.830254	1.632913	-0.696483
H	-6.288829	2.641164	-0.592335
H	-6.388796	0.940987	-0.035157
H	-5.990221	1.308205	-1.745043
C	-3.924030	1.349004	0.955514
H	-4.659803	1.023176	1.708321
C	-2.564032	1.397768	1.315993
C	-2.109363	1.032258	2.706458
H	-1.708296	1.915651	3.250635
H	-1.299791	0.272349	2.673307
H	-2.948044	0.625300	3.304335
C	-1.329581	-1.308183	-0.992779
C	-3.773527	-1.442631	-1.228291
C	-2.643388	-1.573666	-0.376551
C	-5.072654	-1.659079	-0.747302
C	-2.863119	-1.927015	0.978630
C	-5.271731	-2.008780	0.599380
H	-5.933249	-1.547865	-1.425102
C	-4.162010	-2.142802	1.456073
H	-1.993835	-2.016128	1.646976
H	-6.291227	-2.177511	0.981916
H	-4.311711	-2.414718	2.513090
C	-0.163853	-3.038895	-1.012939
C	1.238137	-2.800234	-0.771027
H	-0.740112	-3.576318	-0.241769
H	-0.472867	-3.207737	-2.059111
H	1.666357	-3.179878	0.172997
H	-3.618744	-1.159678	-2.281934
H	-1.428523	-1.110276	-2.084792
H	1.918701	-2.717754	-1.635567

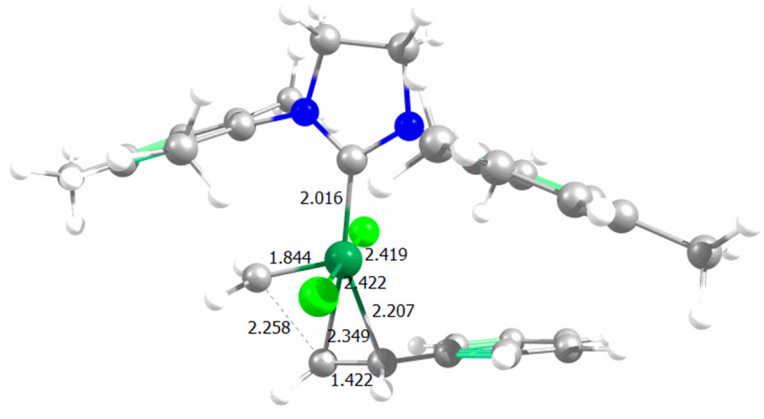
B-MCy1



Zero-point correction =	0.571473 (Hartree/Particle)
Thermal correction to Energy =	0.608400
Thermal correction to Enthalpy =	0.609344
Thermal correction to Gibbs Free Energy =	0.503493
Sum of electronic and zero-point Energies =	−2288.314751
Sum of electronic and thermal Energies =	−2288.277824
Sum of electronic and thermal Enthalpies =	−2288.276879
Sum of electronic and thermal Free Energies =	−2288.382731

Ru	0.309464	-0.856971	-0.332955
Cl	0.126804	-1.708432	1.923024
Cl	0.851446	-0.138075	-2.567928
N	1.988630	1.325559	0.886352
N	-0.170511	1.803597	0.859593
C	0.769945	0.911360	0.473543
C	1.890911	2.525131	1.746934
H	2.640509	3.282895	1.441621
H	2.089391	2.245023	2.804594
C	0.432120	2.980015	1.524240
H	-0.101219	3.206331	2.469140
H	0.352345	3.871866	0.862545
C	3.239656	0.732030	0.497548
C	3.881095	-0.200798	1.347669
C	3.331420	-0.521406	2.715022
H	3.824751	-1.414863	3.145238
H	2.239448	-0.715346	2.681930
H	3.508690	0.322717	3.418102
C	5.078827	-0.786770	0.889894
H	5.582364	-1.528488	1.532294
C	5.651207	-0.447363	-0.351194
C	6.907721	-1.128554	-0.845048
H	7.583997	-0.415181	-1.360068
H	6.658392	-1.925218	-1.580106
H	7.472138	-1.605754	-0.018722
C	5.018140	0.540727	-1.133006
H	5.472426	0.846489	-2.090233
C	3.818848	1.153117	-0.727370
C	3.163815	2.222945	-1.564404
H	3.842043	2.576364	-2.365285
H	2.864086	3.100927	-0.954049
H	2.245440	1.819338	-2.041898
C	-1.552870	1.773583	0.456553
C	-1.904864	2.277198	-0.823366
C	-0.865741	2.785352	-1.790180
H	-1.316499	3.464440	-2.540289
H	-0.389904	1.934418	-2.327252
H	-0.042177	3.327138	-1.282892
C	-3.267744	2.274204	-1.177470
H	-3.556053	2.657767	-2.170652
C	-4.266510	1.812831	-0.298790
C	-5.724086	1.870012	-0.693362
H	-6.126099	2.899967	-0.570926
H	-6.341221	1.192144	-0.071173
H	-5.869054	1.589322	-1.756880
C	-3.877974	1.336419	0.967046
H	-4.646320	0.956917	1.659678
C	-2.531315	1.315777	1.375447
C	-2.145299	0.822881	2.745643
H	-1.614122	1.606330	3.328658
H	-1.456456	-0.046148	2.672699
H	-3.038822	0.518160	3.324094
C	-1.304506	-1.678961	-1.182396
C	-3.746921	-1.333007	-1.361490
C	-2.655713	-1.765523	-0.566191
C	-5.065859	-1.414081	-0.890920
C	-2.930341	-2.256511	0.733938
C	-5.322768	-1.905920	0.399459
H	-5.896183	-1.082811	-1.533473
C	-4.247514	-2.320913	1.208799
H	-2.092693	-2.548906	1.383810
H	-6.356557	-1.963075	0.776337
H	-4.437378	-2.697708	2.226618
C	-0.281161	-2.913107	-1.079561
C	1.224272	-2.562956	-0.775453
H	-0.662165	-3.624008	-0.322865
H	-0.292465	-3.329050	-2.107632
H	1.630538	-3.108492	0.096511
H	-3.548542	-0.932668	-2.368708
H	-1.378341	-1.336908	-2.233771
H	1.881446	-2.536933	-1.664438

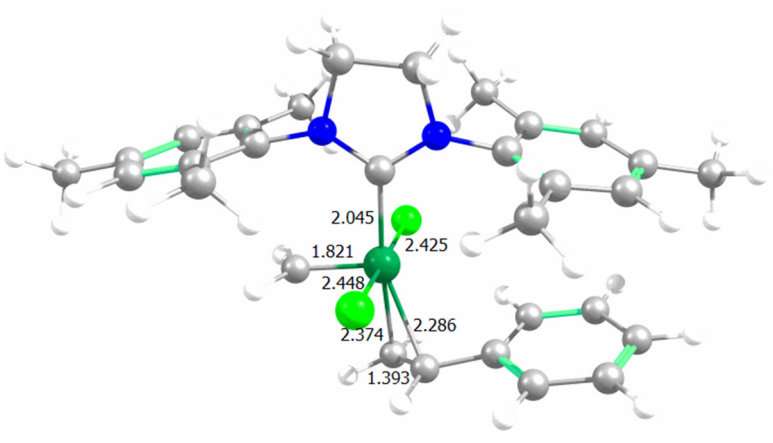
B-MCy1-CI2



Zero-point correction =	0.568790 (Hartree/Particle)
Thermal correction to Energy =	0.606838
Thermal correction to Enthalpy =	0.607782
Thermal correction to Gibbs Free Energy =	0.497561
Sum of electronic and zero-point Energies =	−2288.302131
Sum of electronic and thermal Energies =	−2288.264083
Sum of electronic and thermal Enthalpies =	−2288.263139
Sum of electronic and thermal Free Energies =	−2288.373360

Ru	0.293997	-0.684671	-0.641636
Cl	0.560910	-1.920064	1.421356
Cl	-0.011986	0.549918	-2.702558
N	1.798830	1.459090	0.856008
N	-0.361105	1.890793	0.791332
C	0.597716	1.021941	0.387094
C	1.688113	2.759317	1.549366
H	2.134352	3.563696	0.922152
H	2.232428	2.736519	2.514509
C	0.166341	2.914853	1.717936
H	-0.176908	2.692440	2.753580
H	-0.207971	3.921832	1.443998
C	3.073792	0.861238	0.586324
C	3.685414	0.063455	1.584020
C	3.058080	-0.089274	2.947439
H	3.556160	-0.888644	3.529766
H	1.984138	-0.350703	2.855207
H	3.143225	0.851870	3.534900
C	4.903487	-0.567659	1.265375
H	5.381545	-1.207258	2.025978
C	5.521471	-0.409863	0.008326
C	6.797871	-1.148636	-0.327131
H	7.410599	-1.342477	0.576639
H	7.419710	-0.586174	-1.053167
H	6.571879	-2.136260	-0.786694
C	4.911654	0.442136	-0.934309
H	5.399106	0.607939	-1.909733
C	3.694773	1.099978	-0.667082
C	3.065215	2.021064	-1.681286
H	3.751428	2.209466	-2.529773
H	2.802319	3.002033	-1.232318
H	2.119249	1.597063	-2.086534
C	-1.771823	1.798354	0.537957
C	-2.314805	2.605884	-0.498369
C	-1.415722	3.458494	-1.357445
H	-2.002533	4.069779	-2.070396
H	-0.721109	2.809329	-1.933697
H	-0.793330	4.149100	-0.749017
C	-3.704786	2.572700	-0.701522
H	-4.137489	3.180873	-1.513563
C	-4.558028	1.800413	0.115762
C	-6.046924	1.766562	-0.145297
H	-6.272990	1.181170	-1.063982
H	-6.458687	2.784740	-0.307117
H	-6.602136	1.299818	0.692980
C	-3.985718	1.045040	1.152477
H	-4.635836	0.438511	1.802974
C	-2.594096	1.011508	1.378866
C	-2.033521	0.114904	2.452272
H	-1.037095	0.436240	2.810430
H	-1.883534	-0.911068	2.051659
H	-2.723808	0.045839	3.316458
C	-1.010981	-2.143920	-1.660559
C	-3.302014	-1.587489	-0.902265
C	-2.140761	-2.381231	-0.730491
C	-4.437929	-1.796487	-0.105503
C	-2.142576	-3.378643	0.276985
C	-4.426026	-2.784606	0.892516
H	-5.332475	-1.174629	-0.260011
C	-3.271045	-3.570001	1.082783
H	-1.247591	-3.995059	0.437177
H	-5.315380	-2.947935	1.521855
H	-3.254699	-4.345526	1.864734
C	0.250618	-2.800418	-1.662187
C	1.913962	-1.332657	-1.238635
H	0.508344	-3.536748	-0.884566
H	0.757724	-2.908073	-2.634927
H	2.564593	-1.949207	-0.578456
H	-3.297580	-0.789582	-1.662676
H	-1.301862	-1.654020	-2.606396
H	2.304057	-1.087825	-2.251454

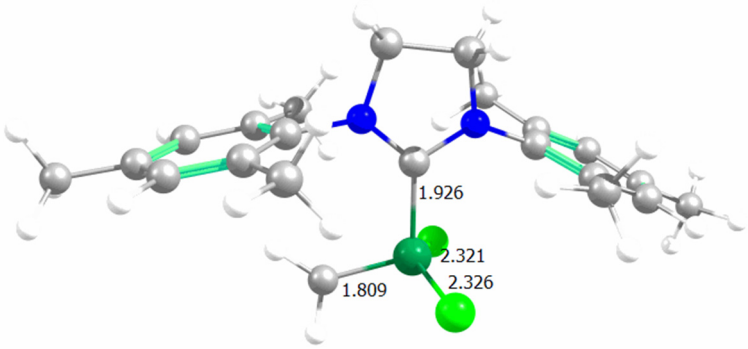
B-CI2



Zero-point correction =	0.568831 (Hartree/Particle)
Thermal correction to Energy =	0.607453
Thermal correction to Enthalpy =	0.608397
Thermal correction to Gibbs Free Energy =	0.498605
Sum of electronic and zero-point Energies =	−2288.306382
Sum of electronic and thermal Energies =	−2288.267760
Sum of electronic and thermal Enthalpies =	−2288.266816
Sum of electronic and thermal Free Energies =	−2288.376608

Ru	-0.295519	-1.074796	-0.371261
Cl	-0.087815	-0.193913	-2.620925
Cl	-0.456692	-1.737336	1.979383
N	-1.860924	1.315622	0.733781
N	0.312299	1.658579	0.775406
C	-0.653267	0.795069	0.374950
C	-1.736776	2.656255	1.345352
H	-2.340965	2.719604	2.271987
H	-2.112774	3.429353	0.637398
C	-0.226111	2.762895	1.599459
H	0.210091	3.730891	1.280964
H	0.041361	2.595229	2.666001
C	-3.162705	0.832730	0.378580
C	-3.668817	1.105954	-0.920124
C	-2.841247	1.836304	-1.944357
H	-3.473798	2.232448	-2.762490
H	-2.076279	1.159438	-2.387845
H	-2.274755	2.680736	-1.501678
C	-4.964172	0.646996	-1.233727
H	-5.363088	0.841327	-2.243291
C	-5.760003	-0.038665	-0.296801
C	-7.131744	-0.557057	-0.664985
H	-7.865667	-0.381242	0.148748
H	-7.103229	-1.654658	-0.842009
H	-7.518715	-0.082122	-1.588693
C	-5.243834	-0.240197	1.000863
H	-5.864783	-0.752390	1.754819
C	-3.958765	0.196168	1.369386
C	-3.434335	-0.009144	2.767186
H	-4.134369	-0.617785	3.372018
H	-3.296957	0.960689	3.294127
H	-2.445054	-0.515350	2.746112
C	1.709867	1.655845	0.439988
C	2.657690	1.157299	1.367134
C	2.231593	0.509941	2.660440
H	3.049254	-0.111520	3.075346
H	1.340777	-0.137940	2.527397
H	1.978096	1.276961	3.426387
C	4.021594	1.330844	1.064331
H	4.770549	0.948811	1.776406
C	4.453597	1.963178	-0.116269
C	5.926173	2.076782	-0.434408
H	6.283774	1.163123	-0.959960
H	6.539169	2.181499	0.484046
H	6.142038	2.939441	-1.096910
C	3.480014	2.449194	-1.010211
H	3.800042	2.961918	-1.932709
C	2.102659	2.330268	-0.745449
C	1.075080	2.928228	-1.673590
H	0.352510	3.572006	-1.127465
H	0.487648	2.122759	-2.166046
H	1.554668	3.543921	-2.459287
C	0.982668	-2.969988	-0.379438
C	3.041904	-2.590537	0.963363
C	2.327929	-2.365964	-0.241050
C	4.368796	-2.161674	1.098403
C	2.954889	-1.623501	-1.276369
C	4.998041	-1.477279	0.042893
H	4.916820	-2.361454	2.032884
C	4.279475	-1.190737	-1.131169
H	2.398910	-1.379135	-2.194460
H	6.042018	-1.141504	0.147164
H	4.752182	-0.615737	-1.942344
C	0.258006	-3.050575	-1.565814
C	-2.042106	-1.540795	-0.593435
H	0.647748	-2.688781	-2.528515
H	-0.623727	-3.706775	-1.616715
H	-2.545170	-1.421117	-1.580064
H	2.538375	-3.118831	1.787752
H	0.651014	-3.565569	0.486057
H	-2.634458	-2.012420	0.221483

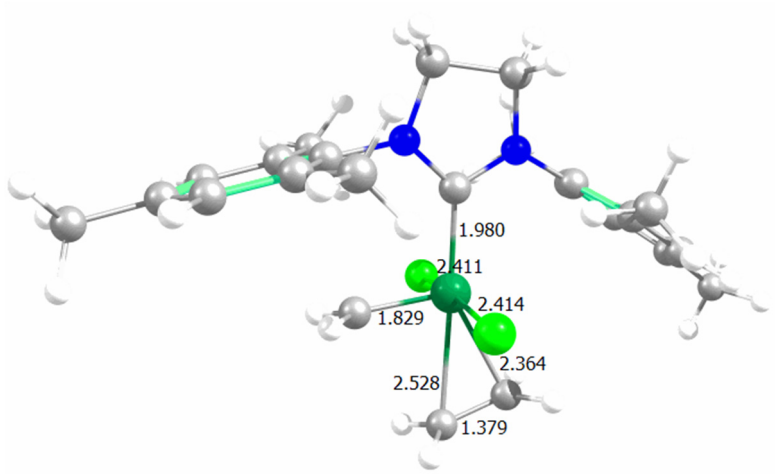
B-14e2



Zero-point correction =	0.436093 (Hartree/Particle)
Thermal correction to Energy =	0.467355
Thermal correction to Enthalpy =	0.468300
Thermal correction to Gibbs Free Energy =	0.372457
Sum of electronic and zero-point Energies =	−1978.974508
Sum of electronic and thermal Energies =	−1978.943246
Sum of electronic and thermal Enthalpies =	−1978.942302
Sum of electronic and thermal Free Energies =	−1979.038145

Ru	-0.092155	0.440236	-1.327866
Cl	-1.095858	-1.491534	-2.134024
Cl	-0.331391	2.733832	-1.022041
N	1.214748	-0.049513	1.328996
N	-0.992146	-0.035735	1.387701
C	0.093219	0.051099	0.548812
C	0.897814	-0.327997	2.741523
H	1.499525	0.320245	3.410598
H	1.139332	-1.387999	2.988019
C	-0.611034	-0.034697	2.808493
H	-1.182936	-0.801095	3.370279
H	-0.830804	0.958571	3.262391
C	2.559735	-0.195492	0.867782
C	3.001252	-1.464860	0.423715
C	2.034318	-2.620385	0.322416
H	2.559932	-3.574372	0.123478
H	1.313138	-2.440670	-0.505982
H	1.425517	-2.746281	1.241247
C	4.332049	-1.577809	-0.024451
H	4.691357	-2.556577	-0.383827
C	5.205216	-0.470364	-0.046592
C	6.639292	-0.620842	-0.502457
H	7.316735	-0.762711	0.368441
H	6.992481	0.280204	-1.044536
H	6.770588	-1.497995	-1.167584
C	4.716474	0.781931	0.382690
H	5.380059	1.662055	0.344672
C	3.396487	0.944807	0.843765
C	2.840921	2.295167	1.223572
H	3.620111	3.080842	1.181621
H	2.411885	2.291534	2.248152
H	2.013058	2.578813	0.537181
C	-2.360100	-0.137221	0.969327
C	-3.172282	1.017063	0.873152
C	-2.695506	2.375726	1.326654
H	-3.011587	3.167651	0.619183
H	-1.594287	2.430953	1.400811
H	-3.133774	2.618722	2.319836
C	-4.493051	0.852727	0.403379
H	-5.131202	1.746542	0.301101
C	-5.016859	-0.409420	0.073053
C	-6.416208	-0.557876	-0.479659
H	-6.941105	-1.427912	-0.033065
H	-6.385868	-0.727695	-1.578247
H	-7.030555	0.347090	-0.300008
C	-4.198751	-1.545367	0.259251
H	-4.604862	-2.546074	0.036524
C	-2.875739	-1.436339	0.713007
C	-2.014924	-2.656402	0.935746
H	-1.625009	-2.696446	1.975862
H	-1.141921	-2.650018	0.252656
H	-2.584693	-3.587357	0.749783
C	1.581026	0.310441	-2.002590
H	2.532552	0.000637	-1.530550
H	1.632070	0.583281	-3.089264

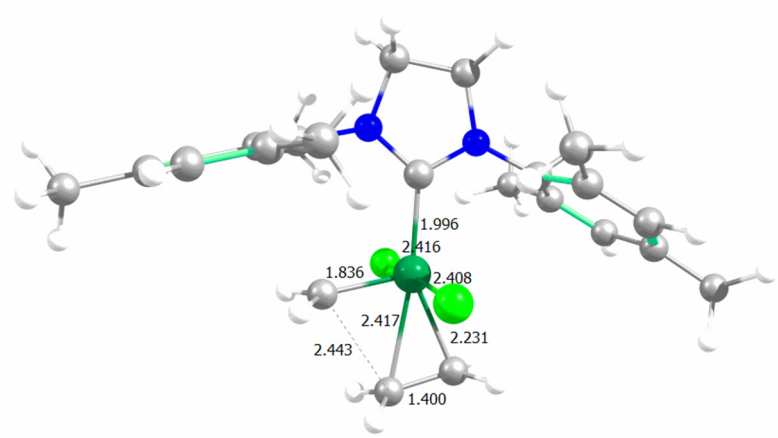
B-CI3



Zero-point correction =	0.489526 (Hartree/Particle)
Thermal correction to Energy =	0.523936
Thermal correction to Enthalpy =	0.524880
Thermal correction to Gibbs Free Energy =	0.421768
Sum of electronic and zero-point Energies =	−2057.475175
Sum of electronic and thermal Energies =	−2057.440765
Sum of electronic and thermal Enthalpies =	−2057.439821
Sum of electronic and thermal Free Energies =	−2057.542933

Ru	-0.209124	1.098993	0.119677
Cl	-0.048927	0.995982	2.526460
Cl	-0.534867	1.499039	-2.235604
N	-0.932763	-1.726214	-0.031030
N	1.267960	-1.565712	0.003425
C	0.110552	-0.850470	-0.014171
C	-0.497682	-3.120580	0.156580
H	-1.020371	-3.798482	-0.548391
H	-0.721272	-3.456121	1.194319
C	1.019421	-3.017989	-0.110002
H	1.629012	-3.579873	0.626030
H	1.297322	-3.374836	-1.127825
C	-2.296337	-1.274533	-0.050332
C	-2.985429	-1.032639	1.166050
C	-2.397296	-1.434501	2.495345
H	-2.877329	-0.885690	3.328530
H	-1.311971	-1.221374	2.546979
H	-2.559371	-2.521282	2.672713
C	-4.276307	-0.471041	1.086224
H	-4.817002	-0.257153	2.023272
C	-4.894313	-0.191139	-0.147753
C	-6.258497	0.458182	-0.209938
H	-6.897952	-0.010947	-0.986328
H	-6.169301	1.534850	-0.473710
H	-6.790839	0.396551	0.760309
C	-4.209918	-0.529575	-1.334172
H	-4.697520	-0.357805	-2.308200
C	-2.917732	-1.082862	-1.313460
C	-2.201385	-1.460915	-2.584041
H	-2.893120	-1.459300	-3.448755
H	-1.738026	-2.466747	-2.509009
H	-1.390453	-0.728678	-2.788005
C	2.584780	-1.012839	-0.087620
C	3.086569	-0.618805	-1.353786
C	2.247008	-0.760131	-2.597746
H	2.856565	-0.621954	-3.511865
H	1.426176	-0.006638	-2.610158
H	1.756892	-1.753848	-2.657707
C	4.376455	-0.050124	-1.400838
H	4.778846	0.269367	-2.376554
C	5.158169	0.119534	-0.242326
C	6.531563	0.749756	-0.306352
H	6.550454	1.716831	0.241246
H	6.848570	0.947012	-1.349670
H	7.296520	0.098608	0.167416
C	4.629470	-0.305695	0.995952
H	5.231426	-0.179977	1.911627
C	3.349129	-0.876979	1.100224
C	2.763946	-1.274934	2.430535
H	2.418600	-2.330794	2.432395
H	1.874240	-0.645002	2.658178
H	3.501364	-1.155972	3.248124
C	1.516157	1.696572	0.004242
C	-1.688999	2.917469	0.418688
C	-0.486920	3.592621	0.429143
H	-2.287306	2.853401	-0.505499
H	-2.155809	2.598044	1.366507
H	-0.090938	4.048841	-0.492963
H	1.925731	2.104569	-0.948346
H	0.041016	3.792382	1.375835
H	2.191002	1.714145	0.889736

B-CI3-MCy2



Zero-point correction = 0.488726 (Hartree/Particle)

Thermal correction to Energy = 0.522430

Thermal correction to Enthalpy = 0.523374

Thermal correction to Gibbs Free Energy = 0.422700

Sum of electronic and zero-point Energies = −2057.472942

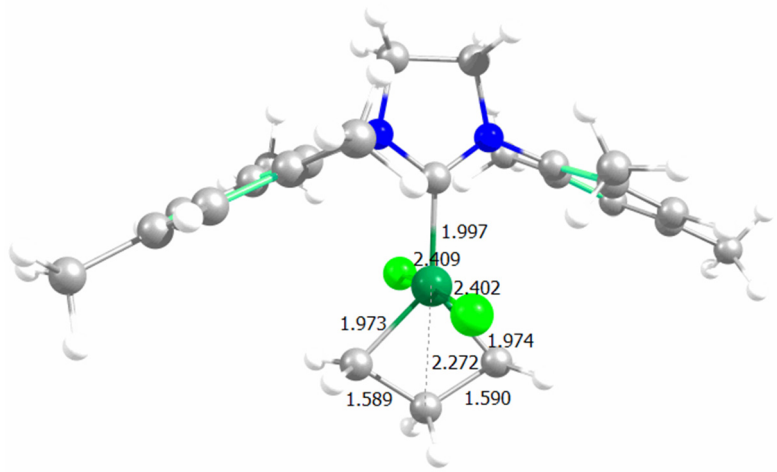
Sum of electronic and thermal Energies = −2057.439239

Sum of electronic and thermal Enthalpies = −2057.438295

Sum of electronic and thermal Free Energies = −2057.538969

Ru	0.147635	-1.139642	-0.116081
Cl	0.554988	-1.468803	2.234679
Cl	-0.112910	-1.054857	-2.516146
N	1.013257	1.685382	-0.084414
N	-1.190970	1.585042	-0.046370
C	-0.051283	0.844187	-0.031961
C	0.610017	3.088296	-0.294677
H	0.824442	3.395727	-1.342575
H	1.165380	3.765448	0.385657
C	-0.904187	3.035136	0.000844
H	-1.159084	3.440923	1.006182
H	-1.511369	3.580223	-0.749568
C	2.371253	1.220965	-0.012687
C	2.964786	1.094048	1.270789
C	2.216022	1.518098	2.508473
H	2.885811	1.550193	3.389713
H	1.401443	0.792280	2.719834
H	1.753104	2.519735	2.386973
C	4.262980	0.558730	1.346438
H	4.729772	0.438718	2.338235
C	4.978177	0.174698	0.193285
C	6.347970	-0.454562	0.312804
H	6.926885	-0.366399	-0.628501
H	6.261706	-1.538081	0.548895
H	6.940597	0.007331	1.129233
C	4.382303	0.384066	-1.065800
H	4.945865	0.131100	-1.979386
C	3.086043	0.922099	-1.200875
C	2.505032	1.220218	-2.560343
H	3.131904	0.788650	-3.364789
H	2.452884	2.317787	-2.733507
H	1.482177	0.802565	-2.669287
C	-2.522002	1.069616	0.084145
C	-3.320174	0.938747	-1.081547
C	-2.772876	1.327618	-2.430962
H	-3.523717	1.171924	-3.229952
H	-1.871263	0.719880	-2.667006
H	-2.465282	2.395087	-2.458914
C	-4.610916	0.399832	-0.937007
H	-5.238912	0.278638	-1.835688
C	-5.119580	0.006054	0.319552
C	-6.509229	-0.581530	0.427103
H	-7.272270	0.112472	0.014327
H	-6.784469	-0.804925	1.477012
H	-6.588814	-1.525943	-0.153110
C	-4.306489	0.177212	1.455833
H	-4.693992	-0.112318	2.446890
C	-3.004532	0.713369	1.368140
C	-2.138414	0.859954	2.593240
H	-1.585478	1.821804	2.599741
H	-1.364800	0.059049	2.630727
H	-2.741362	0.802251	3.520412
C	-1.561293	-1.789697	0.055205
C	0.094192	-3.547497	-0.315755
C	1.367446	-2.979587	-0.439263
H	-0.224460	-3.977217	0.648055
H	-0.478188	-3.817134	-1.218489
H	2.049718	-2.982402	0.427336
H	-2.238419	-1.893065	-0.822312
H	1.795484	-2.820117	-1.443441
H	-1.964037	-2.101148	1.045457

B-MCy2



Zero-point correction =	0.491415 (Hartree/Particle)
Thermal correction to Energy =	0.524180
Thermal correction to Enthalpy =	0.525124
Thermal correction to Gibbs Free Energy =	0.425495
Sum of electronic and zero-point Energies =	−2057.487024
Sum of electronic and thermal Energies =	−2057.454258
Sum of electronic and thermal Enthalpies =	−2057.453314
Sum of electronic and thermal Free Energies =	−2057.552944

Ru	-0.043028	1.103910	0.090147
Cl	0.245023	1.025252	2.481023
Cl	-0.337349	1.384601	-2.277664
N	-1.062993	-1.690151	0.038048
N	1.147603	-1.646332	0.012473
C	0.026940	-0.890451	0.014406
C	-0.693309	-3.113964	0.184864
H	-1.247944	-3.738169	-0.544602
H	-0.946652	-3.469250	1.207847
C	0.831794	-3.089411	-0.068257
H	1.406689	-3.657108	0.690626
H	1.106851	-3.483067	-1.072174
C	-2.412500	-1.192312	0.003307
C	-3.083256	-0.893331	1.215441
C	-2.453928	-1.194753	2.551754
H	-3.114600	-0.881285	3.383320
H	-1.483582	-0.665001	2.667207
H	-2.261916	-2.283084	2.671142
C	-4.366121	-0.317446	1.127082
H	-4.896007	-0.064157	2.060469
C	-4.988472	-0.064515	-0.111310
C	-6.341872	0.606314	-0.180769
H	-6.969957	0.178336	-0.989138
H	-6.230563	1.691542	-0.397775
H	-6.897304	0.515874	0.774376
C	-4.315094	-0.444046	-1.290451
H	-4.803678	-0.288744	-2.266827
C	-3.031531	-1.019441	-1.260887
C	-2.326483	-1.430189	-2.528304
H	-3.017381	-1.414315	-3.393517
H	-1.895359	-2.450249	-2.449740
H	-1.491045	-0.727661	-2.738602
C	2.480862	-1.113141	-0.082080
C	2.993425	-0.749872	-1.353864
C	2.197422	-0.966488	-2.615849
H	2.850295	-0.924979	-3.509521
H	1.409430	-0.187545	-2.724450
H	1.676019	-1.945704	-2.616831
C	4.274141	-0.164694	-1.400013
H	4.682041	0.137379	-2.379250
C	5.046255	0.036062	-0.238879
C	6.427014	0.647331	-0.327692
H	7.187124	-0.125595	-0.577719
H	6.733519	1.111349	0.631466
H	6.479931	1.422481	-1.119365
C	4.522656	-0.393120	0.997327
H	5.123827	-0.265531	1.912978
C	3.248175	-0.981394	1.102782
C	2.707919	-1.446242	2.430968
H	2.421395	-2.519544	2.404111
H	1.800530	-0.863887	2.700265
H	3.457838	-1.317309	3.235482
C	1.245013	2.599237	0.060311
C	-0.131568	3.367479	0.266692
C	-1.439951	2.470554	0.362318
H	-0.048278	3.903566	1.232052
H	-0.261223	4.029753	-0.611322
H	-1.906867	2.473258	1.364988
H	1.715964	2.792318	-0.921814
H	-2.135813	2.602926	-0.487282
H	1.922024	2.656258	0.933002