

# Supplementary Materials: Moving from Classical Ru-NHC to Neutral or Charged Rh-NHC Based Catalysts in Olefin Metathesis

Albert Poater

**Table S1.** Coordinate data sets and absolute energy (in a.u.), 3D structure for DFT optimized complexes with selected distances (in Å).

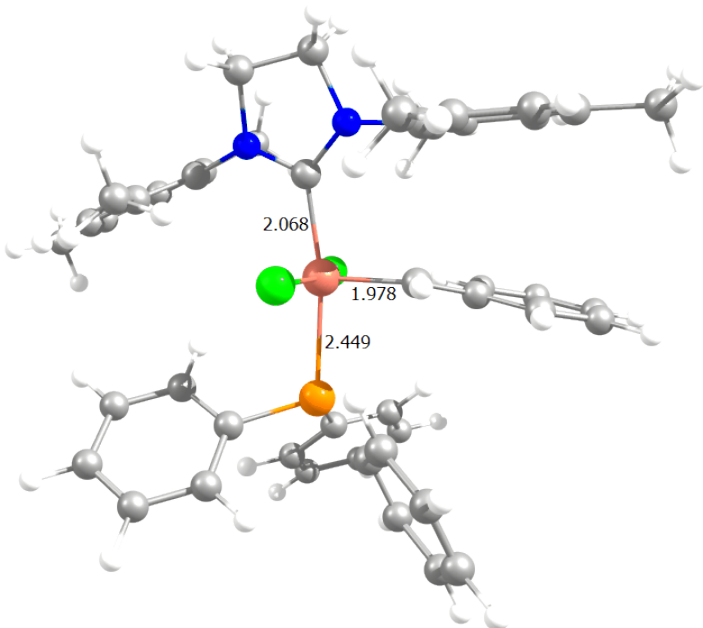
Rh-Id			
			
	Zero-point correction=	0.779957 (Hartree/Particle)	
	Thermal correction to Energy=	0.834865	
	Thermal correction to Enthalpy=	0.835809	
	Thermal correction to Gibbs Free Energy=	0.685232	
	Sum of electronic and Zero-point Energies=	-3263.132801	
	Sum of electronic and thermal Energies=	-3263.077893	
	Sum of electronic and thermal Enthalpies=	-3263.076949	
	Sum of electronic and thermal Free Energies=	-3263.227526	
			Rh -0.081000 -0.296782 -0.126953
			Cl -0.477917 -0.421104 2.199729
			Cl -0.221082 -0.374741 -2.527061
			P -1.077924 1.938544 -0.199992
			N -0.487270 -3.288433 -0.240540
			N 1.641657 -2.843821 -0.553314
			C 0.441845 -2.294336 -0.248220
			C 0.066645 -4.590487 -0.691824
			H -0.317711 -4.825917 -1.697274
			H -0.237514 -5.392401 -0.004293
			C 1.573874 -4.324249 -0.687208
			H 2.090737 -4.794419 0.165871
			H 2.071748 -4.644314 -1.612431
			C -1.873802 -3.242640 0.156830
			C -2.187479 -3.521536 1.509464
			C -1.114511 -3.805088 2.528961
			H -1.563728 -4.106087 3.485389
			H -0.498851 -2.909530 2.702007
			H -0.443776 -4.616149 2.201855
			C -3.534998 -3.552509 1.886349
			H -3.780206 -3.751846 2.933747
			C -4.570993 -3.354578 0.961793
			C -6.014470 -3.362905 1.406553
			H -6.697388 -3.497519 0.555397
			H -6.280677 -2.413846 1.901040
			H -6.207513 -4.168806 2.130852
			C -4.225966 -3.154386 -0.379196
			H -5.017878 -3.044846 -1.126236
			C -2.890320 -3.113848 -0.814096
			C -2.592932 -3.002129 -2.287914
			H -3.463535 -2.602300 -2.826137
			H -2.374881 -3.996004 -2.716629
			H -1.736097 -2.345886 -2.494002
			C 2.959347 -2.266298 -0.479471
			C 3.658149 -1.996756 -1.673954
			C 3.011591 -2.169514 -3.026008
			H 3.637110 -1.722139 -3.811218
			H 2.015426 -1.702241 -3.060798
			H 2.883586 -3.235702 -3.281909
			C 4.985055 -1.553834 -1.572194
			H 5.532175 -1.324359 -2.491827
			C 5.627129 -1.400489 -0.336637
			C 7.039807 -0.875053 -0.253840
			H 7.607088 -1.366053 0.551087
			H 7.036775 0.206441 -0.037855

Table S1. Cont.

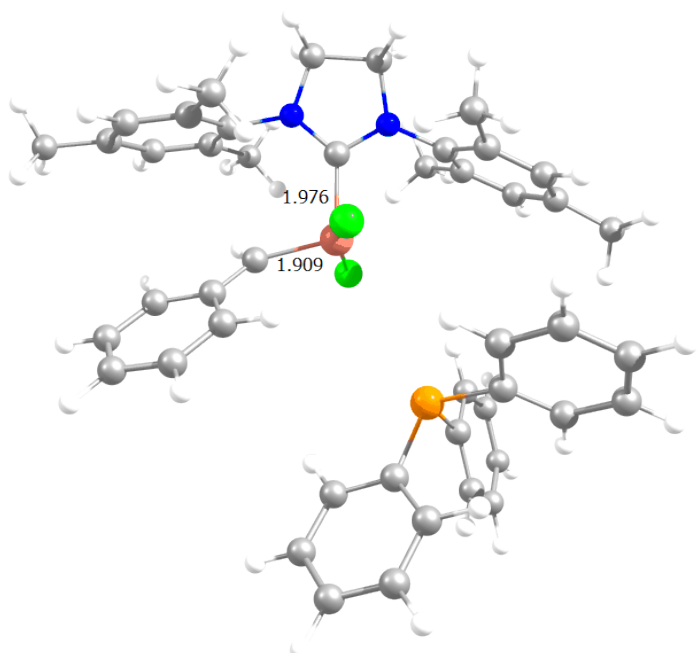
Rh-I-IId					
		Rh	-0.985901	-0.246268	0.169513
		Cl	-0.577599	0.144601	-2.134692
		Cl	-0.673716	-0.639660	2.461642
		P	3.076358	0.935030	0.129291
		N	-2.099520	-2.870218	-0.447574
		N	-3.738636	-1.394354	-0.365180
		C	-2.404522	-1.568317	-0.211365
		C	-3.276347	-3.658189	-0.886981
		H	-3.371257	-4.569729	-0.279396
		H	-3.156331	-3.952439	-1.941408
		C	-4.436259	-2.669687	-0.679470
		H	-5.058498	-2.544593	-1.576954
		H	-5.092655	-2.951711	0.159324
		C	-0.798653	-3.482494	-0.320704
		C	0.026702	-3.627351	-1.458786
		C	-0.436584	-3.245702	-2.841893
		H	0.414463	-3.214328	-3.535633
		H	-0.920617	-2.259406	-2.859123
		H	-1.149465	-3.992114	-3.233731
		C	1.294592	-4.200279	-1.280792
H	1.956298	-4.281805	-2.147561		
C	1.730357	-4.674856	-0.037432		
C	3.125818	-5.220527	0.144108		
H	3.144667	-6.048212	0.868795		
H	3.798389	-4.434204	0.526363		
H	3.546556	-5.580828	-0.805481		
C	0.837948	-4.617825	1.042087		
H	1.137421	-5.034070	2.008410		
C	-0.432506	-4.040053	0.927254		
C	-1.366780	-4.033196	2.110012		
H	-0.982980	-4.690652	2.902414		
H	-2.375839	-4.383015	1.840712		
H	-1.461236	-3.017068	2.524546		
C	-4.541717	-0.232185	-0.094030		
C	-5.041742	-0.035872	1.209913		
C	-4.630701	-0.926627	2.356991		
H	-5.123467	-0.609962	3.286347		
H	-3.540611	-0.897484	2.521434		
H	-4.901166	-1.980691	2.181896		
C	-5.908857	1.046032	1.425609		
H	-6.298060	1.213019	2.434384		
C	-6.286766	1.912007	0.390958		
C	-7.236891	3.059206	0.641823		
H	-8.208060	2.884537	0.150378		
H	-6.836524	4.003389	0.24160		
Zero-point correction=	0.778221 (Hartree/Particle)				
Thermal correction to Energy=	0.831605				
Thermal correction to Enthalpy=	0.832550				
Thermal correction to Gibbs Free Energy=	0.681747				
Sum of electronic and Zero-point Energies=	-3263.111957				
Sum of electronic and thermal Energies=	-3263.058573				
Sum of electronic and thermal Enthalpies=	-3263.057628				
Sum of electronic and thermal Free Energies=	-3263.208431				

Table S1. Cont.

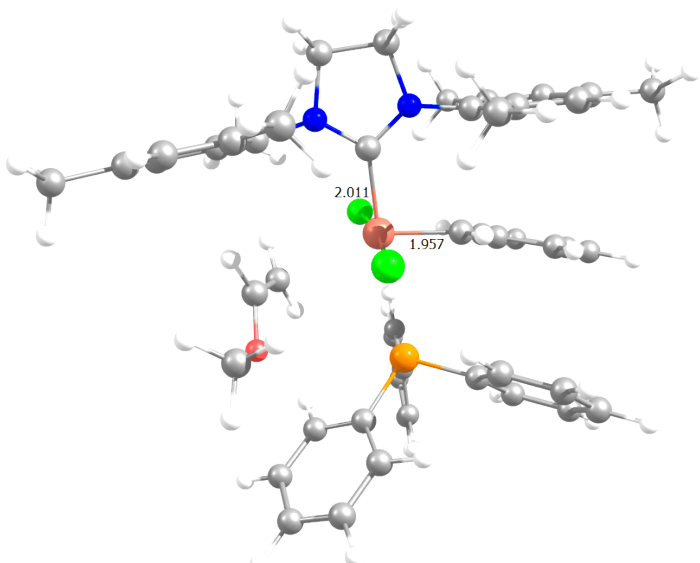
Rh-I-IIIId					
		Rh	0.587676	0.181623	0.157655
		Cl	0.455828	0.477751	2.543819
		Cl	0.903182	-0.371580	-2.166776
		P	-1.811756	-1.932414	0.022525
		N	3.332689	1.422582	0.407304
		N	1.792691	2.961690	0.104301
		C	1.996737	1.616604	0.177107
		C	4.060451	2.695593	0.652835
		H	4.994152	2.710809	0.073671
		H	4.310425	2.776314	1.723234
		C	3.050888	3.744223	0.204125
		H	2.925276	4.563423	0.924823
		H	3.291849	4.181938	-0.779230
		C	4.170376	0.251609	0.355835
		C	4.599475	-0.354618	1.556751
		C	4.100053	0.102295	2.905496
		H	4.238987	-0.688021	3.656605
		H	3.035309	0.379602	2.886515
		H	4.668094	0.981690	3.255687
		C	5.546137	-1.387928	1.476244
		H	5.864739	-1.875495	2.402363
		C	6.103666	-1.797019	0.258356
		C	7.102365	-2.928526	0.202598
		H	7.762978	-2.840055	-0.672171
		H	6.590041	-3.902679	0.131399
		H	7.729440	-2.956767	1.105817
		C	5.695623	-1.134897	-0.908807
		H	6.140267	-1.415772	-1.868249
		C	4.744464	-0.104422	-0.887709
		C	4.367715	0.605513	-2.162106
		H	4.972727	0.237202	-3.002143
		H	4.529255	1.693117	-2.083127
		H	3.302931	0.449549	-2.401363
		C	0.632364	3.755831	-0.212922
		C	0.350311	4.038670	-1.568095
		C	1.102182	3.368932	-2.690850
		H	0.707662	3.693498	-3.663765
		H	1.029403	2.270440	-2.637758
		H	2.175899	3.621185	-2.671508
		C	-0.660894	4.966524	-1.848955
		H	-0.899181	5.179435	-2.895576
		C	-1.361966	5.635168	-0.835403
		C	-2.476485	6.596756	-1.166771
		H	-2.518525	7.430099	-0.449544
		H	-3.451967	6.083266	-1.127960
Zero-point correction=		0.863231 (Hartree/Particle)			
Thermal correction to Energy=		0.923813			
Thermal correction to Enthalpy=		0.924757			
Thermal correction to Gibbs Free Energy=		0.763548			
Sum of electronic and Zero-point Energies=		-3456.200352			
Sum of electronic and thermal Energies=		-3456.139770			
Sum of electronic and thermal Enthalpies=		-3456.138825			
Sum of electronic and thermal Free Energies=		-3456.300034			

Table S1. Cont.

Rh-I+					
Zero-point correction=	0.783437 (Hartree/Particle)	Rh	-0.050729	-0.256585	-0.163370
Thermal correction to Energy=	0.837957	Cl	-0.420070	-0.333458	2.163734
Thermal correction to Enthalpy=	0.838901	Cl	-0.269710	-0.352502	-2.529691
Thermal correction to Gibbs Free Energy=	0.690101	P	-0.883114	2.058449	-0.196842
Sum of electronic and Zero-point Energies=	-3262.949401	N	-0.830600	-3.209052	-0.202109
Sum of electronic and thermal Energies=	-3262.894881	N	1.342647	-2.993335	-0.479954
Sum of electronic and thermal Enthalpies=	-3262.893937	C	0.189592	-2.331052	-0.237308
Sum of electronic and thermal Free Energies=	-3263.042738	C	-0.391926	-4.600158	-0.506859
		H	-0.851836	-4.924938	-1.452237
		H	-0.722444	-5.279061	0.290770
		C	1.134806	-4.465922	-0.595890
		H	1.663259	-4.977904	0.222731
		H	1.541668	-4.827425	-1.550026
		C	-2.221477	-2.997416	0.131642
		C	-2.620360	-3.208088	1.476726
		C	-1.637647	-3.588277	2.556279
		H	-2.113019	-3.528544	3.544453
		H	-0.759242	-2.929975	2.563613
		H	-1.287797	-4.627290	2.429356
		C	-3.980747	-3.109955	1.782305
		H	-4.294763	-3.257033	2.819718
		C	-4.952803	-2.868860	0.796845
		C	-6.417598	-2.820202	1.160204
		H	-7.033377	-2.479053	0.316482
		H	-6.598805	-2.149347	2.014142
		H	-6.782232	-3.817567	1.454635
		C	-4.525899	-2.720914	-0.525425
		H	-5.268048	-2.563750	-1.313379
		C	-3.170262	-2.795282	-0.891662
		C	-2.805989	-2.689472	-2.351880
		H	-2.919386	-1.655550	-2.711314
		H	-3.470428	-3.326313	-2.954993
		H	-1.766527	-2.974527	-2.552055
		C	2.698425	-2.517287	-0.426630
		C	3.408398	-2.319100	-1.634693
		C	2.745526	-2.477001	-2.979860
		H	3.372511	-2.048398	-3.773414
		H	1.758686	-1.991643	-3.011566
		H	2.598618	-3.541928	-3.227940
		C	4.768358	-1.988935	-1.549556
		H	5.325665	-1.825768	-2.476516
		C	5.438662	-1.895263	-0.320892
		C	6.917588	-1.604862	-0.263801
		H	7.491501	-2.540258	-0.156861
		H	7.172279	-0.970212	0.597505

Table S1. Cont.

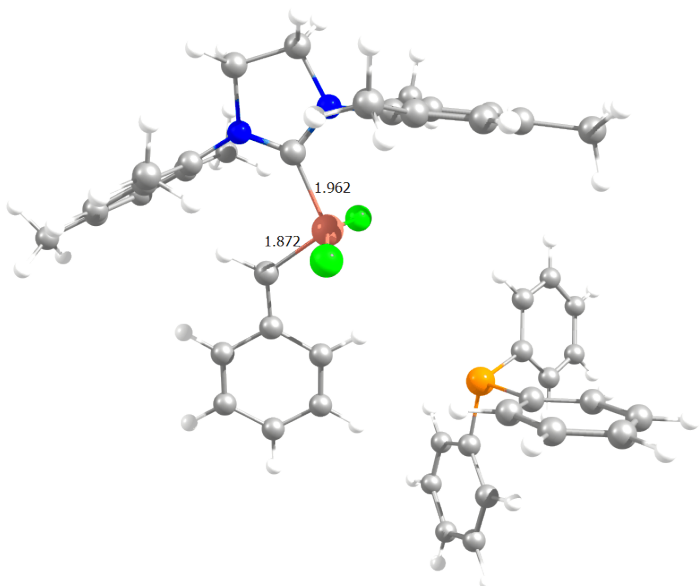
Rh-I-II+					
		Rh	-1.517368	-0.193701	-0.112379
		Cl	-1.324664	-0.473538	-2.391064
Zero-point correction= 0.780723 (Hartree/Particle) Thermal correction to Energy= 0.835908 Thermal correction to Enthalpy= 0.836852 Thermal correction to Gibbs Free Energy= 0.679724 Sum of electronic and Zero-point Energies= -3262.913128 Sum of electronic and thermal Energies= -3262.857944 Sum of electronic and thermal Enthalpies= -3262.857000 Sum of electronic and thermal Free Energies= -3263.014127		Cl	-0.906156	-0.190625	2.106926
		P	3.929997	0.537466	0.112358
		N	-3.239060	-2.418593	0.209903
		N	-4.499624	-0.596888	0.297493
		C	-3.252012	-1.074666	0.142879
		C	-4.597047	-2.975932	0.434463
		H	-4.609874	-3.548104	1.373093
		H	-4.860392	-3.649456	-0.393421
		C	-5.478057	-1.711112	0.487450
		H	-6.229273	-1.675513	-0.314001
		H	-5.990392	-1.584638	1.451184
		C	-2.076434	-3.264953	0.050842
		C	-1.767405	-3.769563	-1.236587
		C	-2.652568	-3.545047	-2.438000
		H	-2.051606	-3.415397	-3.347977
		H	-3.293868	-2.661673	-2.339521
		H	-3.298835	-4.425603	-2.595914
		C	-0.632114	-4.577457	-1.364540
		H	-0.368891	-4.953920	-2.356821
		C	0.162080	-4.930966	-0.263632
		C	1.408235	-5.759987	-0.443771
		H	1.643476	-6.337915	0.460935
		H	2.274457	-5.111480	-0.655414
		H	1.310231	-6.458584	-1.286820
		C	-0.235870	-4.493676	1.007224
		H	0.336509	-4.807454	1.884552
		C	-1.362657	-3.683925	1.200076
		C	-1.820324	-3.380335	2.605406
		H	-0.964684	-3.165947	3.259967
		H	-2.339186	-4.259259	3.024828
		H	-2.498881	-2.521720	2.659355
		C	-4.997537	0.754638	0.262239
		C	-5.136457	1.464999	1.474842
		C	-4.690884	0.882320	2.793824
		H	-4.817805	1.615658	3.600784
		H	-3.632528	0.579538	2.772447
		H	-5.280338	-0.008178	3.066917
		C	-5.690844	2.751534	1.415177
		H	-5.800721	3.316688	2.344831
		C	-6.118576	3.325805	0.207972
		C	-6.762936	4.689979	0.186992
		H	-6.633267	5.185831	-0.785258
		H	-6.352522	5.343977	0.969521

Table S1. Cont.

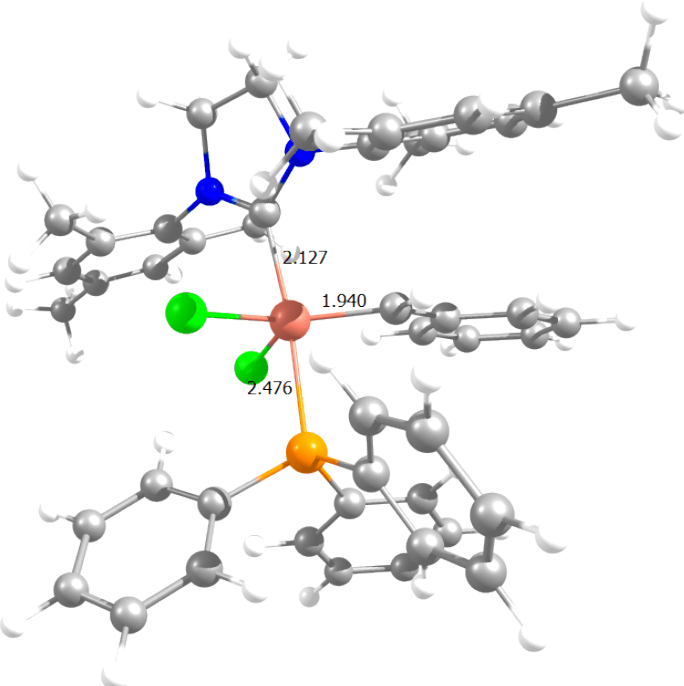
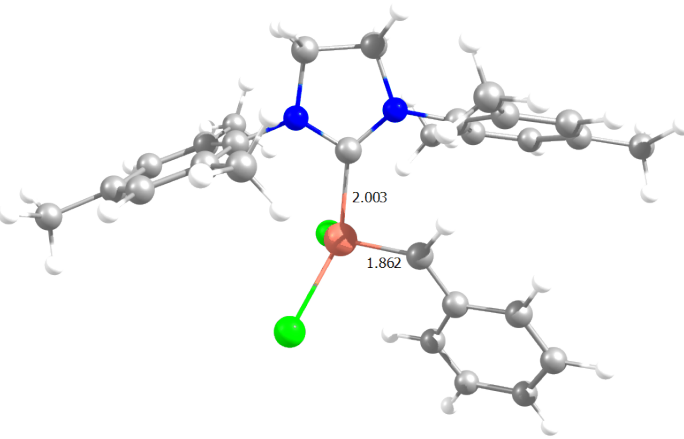
Rh-I+†		
		Rh -0.234067 -0.100321 -0.197577
		Cl -1.778818 0.767088 1.439337
<p>Zero-point correction= 0.781943 (Hartree/Particle)            Thermal correction to Energy= 0.837034            Thermal correction to Enthalpy= 0.837978            Thermal correction to Gibbs Free Energy= 0.685530            Sum of electronic and Zero-point Energies= -3262.899720            Sum of electronic and thermal Energies= -3262.844629            Sum of electronic and thermal Enthalpies= -3262.843685            Sum of electronic and thermal Free Energies= -3262.996133</p>		Cl -0.979925 0.342182 -2.428167
		P 0.686361 2.197519 -0.243629
<p>Zero-point correction= 0.513724 (Hartree/Particle)            Thermal correction to Energy= 0.550901            Thermal correction to Enthalpy= 0.551845            Thermal correction to Gibbs Free Energy= 0.439856            Sum of electronic and Zero-point Energies= -2226.842365            Sum of electronic and thermal Energies= -2226.805188            Sum of electronic and thermal Enthalpies= -2226.804244            Sum of electronic and thermal Free Energies= -2226.916232</p>		N -2.413549 -2.339734 -0.511378
		N -0.384007 -3.086925 -0.913710
		C -1.103844 -2.021913 -0.475330
		C -2.652171 -3.727367 -1.003816
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -3.325451 -3.696124 -1.871148
		H -3.136556 -4.315899 -0.210131
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -2.016753 -1.955723 2.429859
		H -2.769418 -3.507082 1.996746
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		C -3.883752 -1.744742 1.362771
		C -2.980936 -2.476373 2.324249
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -3.443247 -2.533126 3.318744
		H -3.443247 -2.533126 3.318744
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -5.059375 -1.146805 1.824439
		H -5.059375 -1.146805 1.824439
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -5.300367 -1.216876 2.888987
		H -5.300367 -1.216876 2.888987
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		C -5.935970 -0.466365 0.964021
		C -5.935970 -0.466365 0.964021
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		C -7.178386 0.202103 1.499753
		C -7.178386 0.202103 1.499753
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl -1.371397 2.960110 -0.610706            N -1.719370 -1.692714 -0.060106            N 0.441263 -2.104507 -0.104966            C -0.489865 -1.110293 -0.056844            C -1.665718 -3.162152 -0.230512            H -2.013315 -3.434827 -1.241995            H -2.312510 -3.664118 0.502550            C -0.174713 -3.455868 -0.017494            H 0.032008 -3.890121 0.974713            H 0.246966 -4.124233 -0.781358            C -2.974609 -0.989603 -0.149204            C -3.780632 -0.897709 1.006962            C -3.313830 -1.430816 2.337031            H -4.084875 -1.278495 3.104647            H -2.396813 -0.909951 2.658298            H -3.089870 -2.509414 2.297773            C -5.023520 -0.261229 0.893843            H -5.647893 -0.170835 1.787418            C -5.481383 0.267758 -0.320275            C -6.801681 0.995679 -0.399190            H -7.262435 0.890357 -1.392391            H -6.660848 2.073838 -0.215478            H -7.512968 0.624240 0.352879            C -4.666945 0.132599 -1.452442            H -5.009706 0.532766 -2.410996            C -3.415987 -0.495031 -1.396752            C -2.567751 -0.595599 -2.640983            H -3.170720 -0.390710 -3.536399            H -2.109790 -1.589849 -2.756508            H -1.747968 0.141822 -2.611006            C 1.873795 -2.007239 -0.019892            C 2.628922 -2.189548 -1.199288            C 1.959707 -2.396541 -2.537636            H 2.696723 -2.351221 -3.351152</p>		H -7.901687 0.410604 0.699188
		H -7.901687 0.410604 0.699188
<p>Rh -0.450891 0.892069 -0.009599            Cl -0.651052 1.048563 2.383255            Cl</p>		

Table S1. Cont.

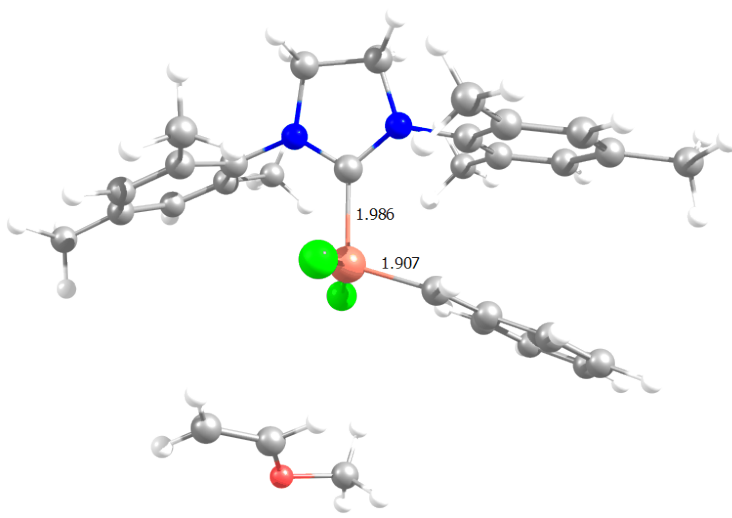
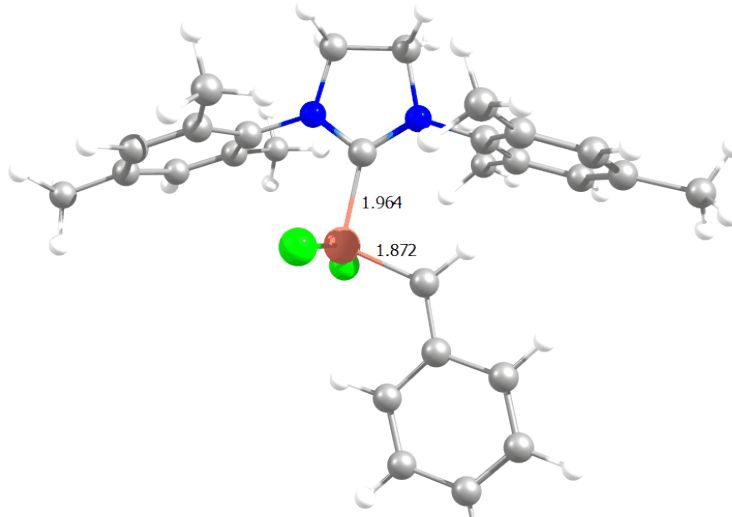
Rh-II-IIIId					
		Rh	-0.378117	0.515141	-0.332847
		Cl	-0.704031	1.433532	1.798442
		Cl	-0.689001	0.221004	-2.660956
		N	-1.549371	-2.109715	0.285621
		N	0.636092	-2.306693	0.055918
		C	-0.396186	-1.431155	0.061232
		C	-1.337479	-3.577051	0.344874
		H	-1.778370	-4.053883	-0.544870
		H	-1.820028	-3.994601	1.240008
		C	0.195480	-3.690340	0.374731
		H	0.581579	-3.984922	1.364196
		H	0.589253	-4.393401	-0.372414
		C	-2.876945	-1.552995	0.393405
		C	-3.352305	-1.186796	1.673682
		C	-2.510459	-1.356407	2.912832
		H	-3.120180	-1.200109	3.813354
		H	-1.686147	-0.626187	2.927860
		H	-2.067840	-2.363240	2.974733
		C	-4.647052	-0.661928	1.770109
		H	-5.016224	-0.357228	2.753620
		C	-5.477890	-0.521768	0.650032
		C	-6.845107	0.105824	0.774176
		H	-7.530156	-0.261150	-0.003835
		H	-6.779280	1.201212	0.665417
		H	-7.295471	-0.098747	1.756585
		C	-5.000192	-0.968454	-0.588346
		H	-5.647610	-0.903992	-1.467634
		C	-3.714855	-1.506846	-0.743764
		C	-3.287299	-2.051511	-2.081890
		H	-3.969873	-1.712625	-2.871616
		H	-3.314934	-3.158756	-2.083266
		H	-2.273223	-1.730978	-2.354655
		C	2.045406	-2.039786	-0.042815
		C	2.688178	-2.218169	-1.284541
		C	1.912344	-2.556851	-2.532767
		H	2.586778	-2.633629	-3.396687
Zero-point correction= 0.596176 (Hartree/Particle) Thermal correction to Energy= 0.639645 Thermal correction to Enthalpy= 0.640589 Thermal correction to Gibbs Free Energy= 0.513000 Sum of electronic and Zero-point Energies= -2419.937562 Sum of electronic and thermal Energies= -2419.894093 Sum of electronic and thermal Enthalpies= -2419.893149 Sum of electronic and thermal Free Energies= -2420.020738					
Rh-II+					
		Rh	-0.349358	0.819152	-0.055858
		Cl	-0.597322	1.240220	2.193698
		Cl	-0.690078	1.077672	-2.317079
		N	-1.734351	-1.645826	0.055610
		N	0.433857	-2.112982	0.068078
		C	-0.489800	-1.137618	0.027995
		C	-1.724274	-3.129467	0.125509
		H	-2.252550	-3.542708	-0.745208
		H	-2.238059	-3.458093	1.040035
		C	-0.216667	-3.458257	0.128886
		H	0.108782	-3.978167	1.040743
		H	0.094455	-4.053216	-0.741031
		C	-2.960738	-0.877376	0.031997
		C	-3.568794	-0.511742	1.258232
		C	-3.054761	-0.974365	2.599168
		H	-3.177240	-0.189153	3.357250
		H	-1.994445	-1.251152	2.581738
		H	-3.635844	-1.848773	2.938864
		C	-4.749023	0.240407	1.201296
		H	-5.215566	0.549595	2.140696
		C	-5.357435	0.585407	-0.013661
		C	-6.601511	1.436535	-0.042809
		H	-7.228483	1.205801	-0.915453
		H	-6.336102	2.505194	-0.103498
		H	-7.205108	1.300813	0.865472
		C	-4.778945	0.114678	-1.201790
		H	-5.269027	0.326978	-2.155911
		C	-3.598947	-0.638226	-1.210613
		C	-3.110514	-1.233245	-2.507984
		H	-3.342114	-0.570031	-3.352033
		H	-3.623015	-2.192251	-2.698123
		H	-2.029349	-1.412825	-2.517993
		C	1.872834	-2.037023	0.060454
		C	2.551915	-2.124735	-1.174649
		C	1.810186	-2.203074	-2.487246
		H	2.515412	-2.204686	-3.328400
Zero-point correction= 0.515783 (Hartree/Particle) Thermal correction to Energy= 0.552809 Thermal correction to Enthalpy= 0.553753 Thermal correction to Gibbs Free Energy= 0.442459 Sum of electronic and Zero-point Energies= -2226.633557 Sum of electronic and thermal Energies= -2226.596532 Sum of electronic and thermal Enthalpies= -2226.595587 Sum of electronic and thermal Free Energies= -2226.706881					

Table S1. Cont.

Rh-III-III+					
Zero-point correction=	0.597836 (Hartree/Particle)	Rh	0.282139	0.039250	-0.121879
Thermal correction to Energy=	0.641679	Cl	0.587040	-0.105473	-2.399544
Thermal correction to Enthalpy=	0.642624	Cl	0.819429	0.398292	2.088405
Thermal correction to Gibbs Free Energy=	0.510695	N	0.096040	-2.769462	0.220685
Sum of electronic and Zero-point Energies=	-2419.735625	N	-1.969710	-1.964686	0.255473
Sum of electronic and thermal Energies=	-2419.691782	C	-0.664843	-1.662930	0.133871
Sum of electronic and thermal Enthalpies=	-2419.690837	C	-0.723905	-3.990730	0.425946
Sum of electronic and thermal Free Energies=	-2419.822766	H	-0.436743	-4.471295	1.372044
		H	-0.545247	-4.696512	-0.397627
		C	-2.162367	-3.435365	0.443187
		H	-2.784368	-3.828450	-0.373115
		H	-2.681388	-3.615746	1.394848
		C	1.536947	-2.827608	0.102900
		C	2.111504	-3.081821	-1.167324
		C	1.285697	-3.382427	-2.393756
		H	1.758859	-2.968959	-3.294388
		H	0.271030	-2.972020	-2.338502
		H	1.211204	-4.474276	-2.536524
		C	3.507439	-3.137762	-1.251604
		H	3.963986	-3.313291	-2.229706
		C	4.331002	-2.999185	-0.124419
		C	5.832804	-3.022629	-0.258281
		H	6.317549	-3.331471	0.678236
		H	6.214970	-2.019975	-0.512410
		H	6.155662	-3.704785	-1.057678
		C	3.719871	-2.844281	1.127270
		H	4.343074	-2.789204	2.024135
		C	2.328146	-2.783229	1.276628
		C	1.735714	-2.770109	2.664122
		H	2.333892	-2.143694	3.339556
		H	1.737788	-3.792203	3.080214
		H	0.708474	-2.389745	2.687224
		C	-3.133993	-1.116650	0.212774
		C	-3.639416	-0.587408	1.420252
		C	-2.940783	-0.809722	2.739413
		H	-3.492704	-0.323645	3.554298
RhIII-ZVP+t					
Zero-point correction=	0.514060 (Hartree/Particle)	Rh	-0.467156	0.785099	0.121855
Thermal correction to Energy=	0.551859	Cl	-0.473555	1.403997	2.355029
Thermal correction to Enthalpy=	0.552803	Cl	-1.490187	2.503882	-1.005465
Thermal correction to Gibbs Free Energy=	0.437697	N	-1.676678	-1.818297	-0.137112
Sum of electronic and Zero-point Energies=	-2226.599591	N	0.490856	-2.230731	-0.131954
Sum of electronic and thermal Energies=	-2226.561792	C	-0.450866	-1.273032	-0.093328
Sum of electronic and thermal Enthalpies=	-2226.560848	C	-1.637021	-3.303342	-0.217606
Sum of electronic and thermal Free Energies=	-2226.675954	H	-2.116014	-3.636396	-1.149893
		H	-2.184085	-3.740417	0.629382
		C	-0.121392	-3.596646	-0.176932
		H	0.183959	-4.159448	0.716898
		H	0.235198	-4.135073	-1.065434
		C	-2.901463	-1.052337	-0.153400
		C	-3.607730	-0.866268	1.058600
		C	-3.110683	-1.421594	2.370868
		H	-3.635745	-0.949380	3.211270
		H	-2.033989	-1.253425	2.513424
		H	-3.295500	-2.506790	2.442291
		C	-4.814309	-0.157968	1.004710
		H	-5.363333	0.011244	1.934872
		C	-5.340787	0.331073	-0.200902
		C	-6.628469	1.113559	-0.219328
		H	-7.164864	0.985816	-1.169999
		H	-6.425567	2.190868	-0.099493
		H	-7.295598	0.813078	0.600661
		C	-4.627066	0.091730	-1.385448
		H	-5.031107	0.452896	-2.334810
		C	-3.410972	-0.598996	-1.393998
		C	-2.676064	-0.827144	-2.692575
		H	-3.331871	-0.613180	-3.546537
		H	-2.318060	-1.862715	-2.795857
		H	-1.801117	-0.162387	-2.777194
		C	1.920612	-2.083224	-0.030888
		C	2.698984	-2.193195	-1.205205
		C	2.073662	-2.416582	-2.562444
		H	2.771895	-2.138923	-3.363227



Table S1. Cont.

RhIII-TZVPd					
		Rh	-0.498155	0.756382	-0.244903
		Cl	-0.622926	1.198779	2.077436
<p>Zero-point correction= 0.597775 (Hartree/Particle)            Thermal correction to Energy= 0.640837            Thermal correction to Enthalpy= 0.641781            Thermal correction to Gibbs Free Energy= 0.517944            Sum of electronic and Zero-point Energies= -2419.945501            Sum of electronic and thermal Energies= -2419.902438            Sum of electronic and thermal Enthalpies= -2419.901494            Sum of electronic and thermal Free Energies= -2420.025331</p>		Cl	-0.706379	0.468594	-2.611890
		N	-1.945036	-1.726795	0.246972
		N	0.191471	-2.236695	0.105725
		C	-0.694850	-1.215074	0.068623
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	-1.953867	-3.207805	0.295416
		H	-2.407022	-3.607084	-0.626716
		H	-2.542129	-3.559789	1.154363
		C	-0.461510	-3.538417	0.411002
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	-0.174387	-3.863705	1.424162
		H	-0.130309	-4.303523	-0.304404
		C	-3.194299	-1.003275	0.254519
		C	-3.759697	-0.638873	1.501266
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	-3.114939	-1.019795	2.809036
		H	-3.702737	-0.632210	3.652418
		H	-2.095686	-0.614393	2.885057
		H	-3.056539	-2.115563	2.921316
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	-4.977445	0.052817	1.497765
		H	-5.408368	0.355114	2.456690
		C	-5.662265	0.351500	0.311110
		C	-6.944547	1.148412	0.335598
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	-7.571019	0.931070	-0.541587
		H	-6.732810	2.230768	0.328974
		H	-7.532864	0.937795	1.240990
		C	-5.124655	-0.114813	-0.893960
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	-5.671857	0.053173	-1.826411
		C	-3.912352	-0.820482	-0.949637
		C	-3.481410	-1.439951	-2.255641
		H	-3.866510	-0.860805	-3.106184
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	-3.894434	-2.460730	-2.341652
		H	-2.391790	-1.487012	-2.361648
		C	1.629581	-2.238338	0.022095
		C	2.228508	-2.573590	-1.209774
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	1.405539	-2.753130	-2.461747
		H	2.055750	-2.953428	-3.324575
RhIII-IVTZVPd					
		Rh	0.004304	-0.825789	-0.160380
		Cl	-0.285416	-0.939484	2.220144
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		Cl	0.617775	-0.708717	-2.470754
		N	1.950225	1.646583	0.188062
		N	-0.174499	2.187357	0.103299
		C	0.695477	1.150180	0.072811
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	1.966820	3.121114	0.403005
		H	2.660984	3.599869	-0.301838
		H	2.308139	3.340782	1.427496
		C	0.502939	3.509074	0.167119
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	0.079177	4.113315	0.981036
		H	0.352266	4.049863	-0.781004
		C	3.215732	0.960137	0.222179
		C	3.729151	0.506357	1.456613
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	2.940034	0.621390	2.735588
		H	3.504599	0.194412	3.576095
		H	1.969059	0.104975	2.668597
		H	2.726743	1.674539	2.983091
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	5.022578	-0.039227	1.473698
		H	5.424942	-0.396339	2.426512
		C	5.817784	-0.111425	0.322553
		C	7.202624	-0.713586	0.368439
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	7.900083	-0.167687	-0.284272
		H	7.191775	-1.762019	0.026428
		H	7.610361	-0.705291	1.389474
		C	5.287833	0.382511	-0.878332
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	5.897044	0.352670	-1.786695
		C	3.998938	0.930026	-0.954968
		C	3.476718	1.463848	-2.264048
		H	4.223537	1.332617	-3.059187
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		H	3.241607	2.539350	-2.203060
		H	2.552557	0.940317	-2.557679
		C	-1.613627	2.153572	-0.007528
		C	-2.215305	2.205659	-1.283789
<p>Zero-point correction= 0.598287 (Hartree/Particle)            Thermal correction to Energy= 0.640080            Thermal correction to Enthalpy= 0.641025            Thermal correction to Gibbs Free Energy= 0.521035            Sum of electronic and Zero-point Energies= -2419.933635            Sum of electronic and thermal Energies= -2419.891842            Sum of electronic and thermal Enthalpies= -2419.890898            Sum of electronic and thermal Free Energies= -2420.010888</p>		C	-1.402127	2.257303	-2.552048
		H	-2.062646	2.356760	-3.424678

Table S1. Cont.

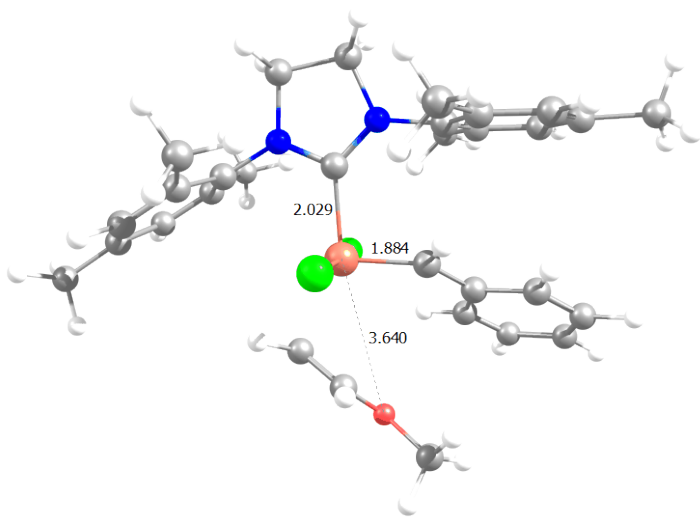
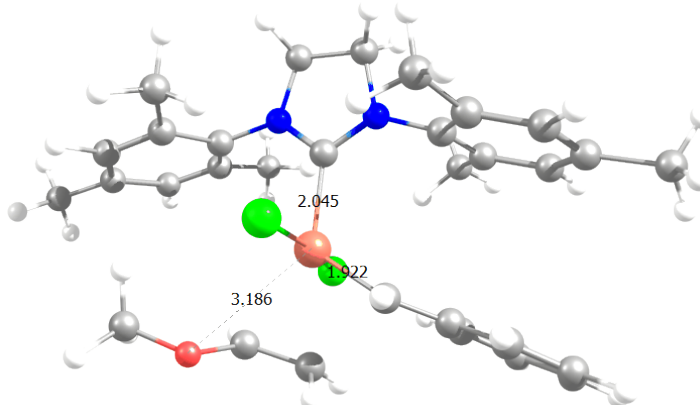
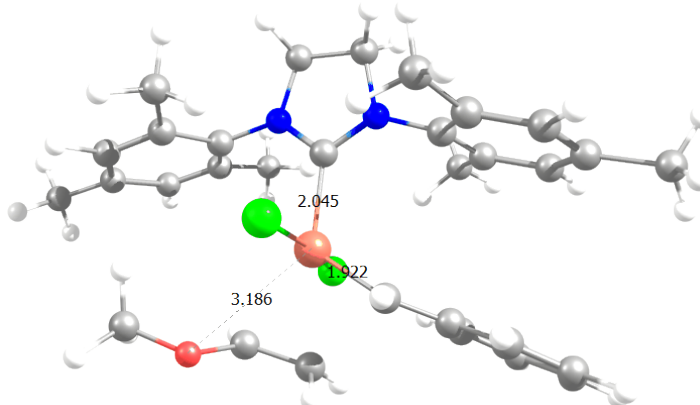
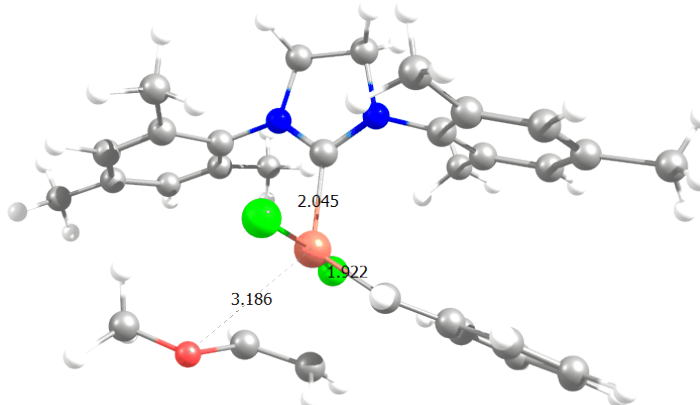
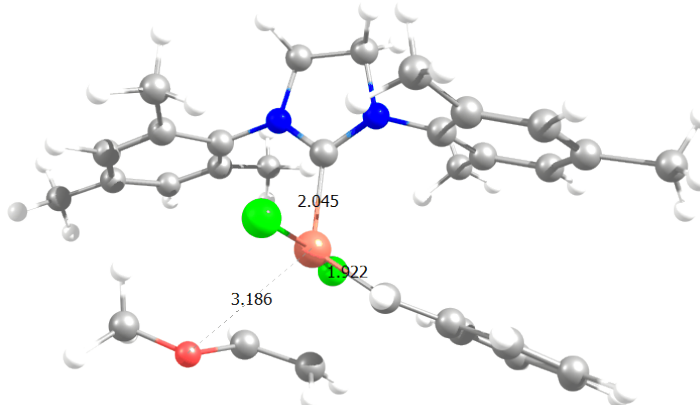
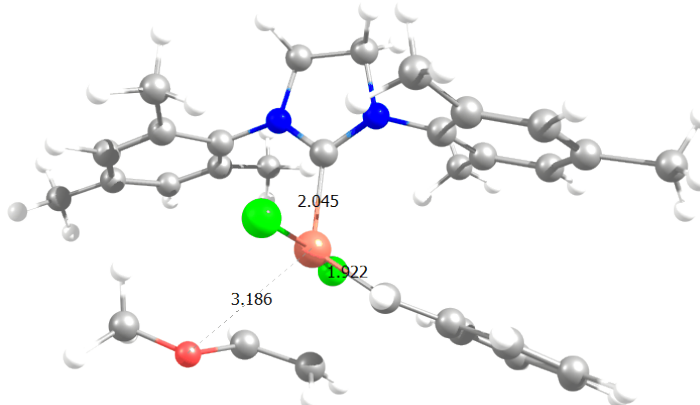
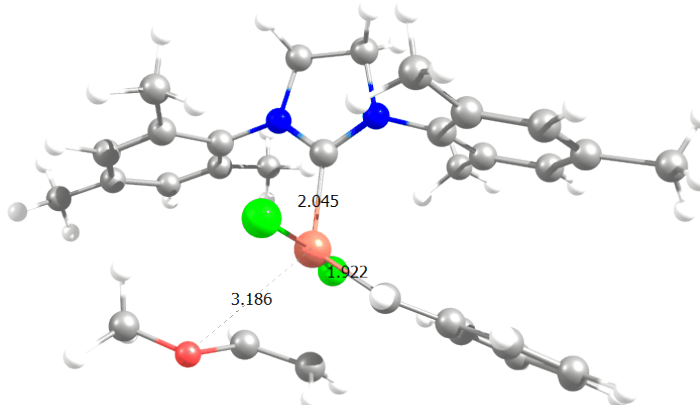
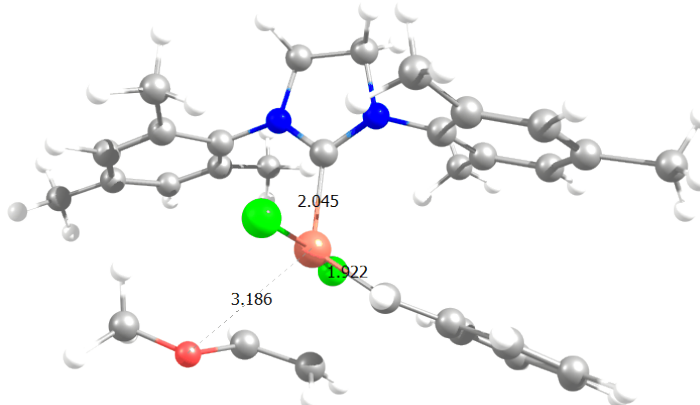
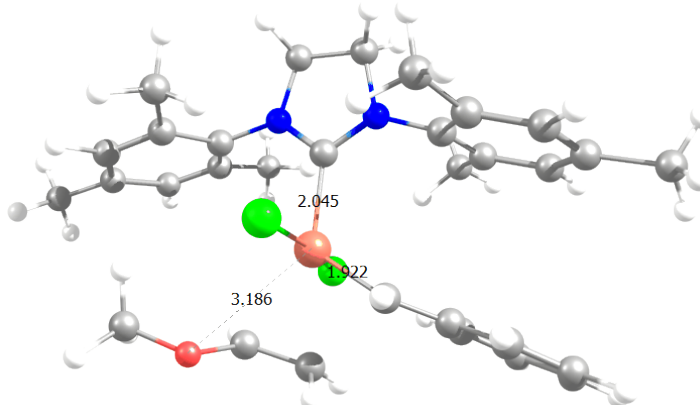
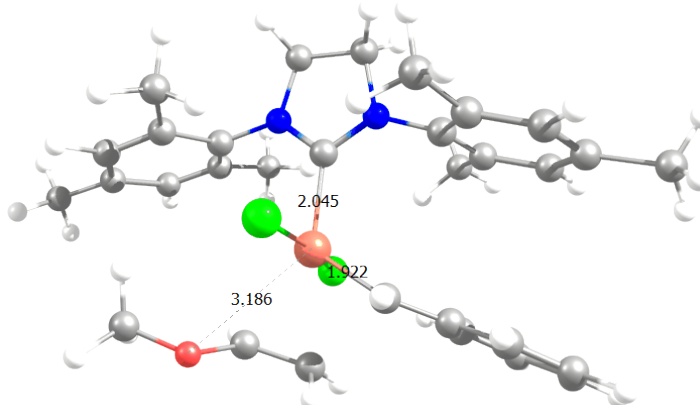
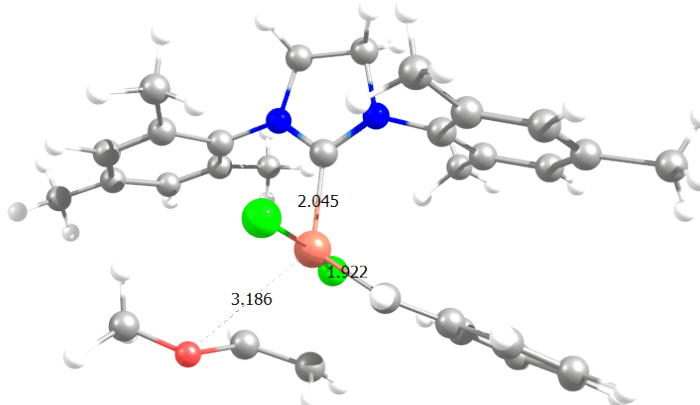
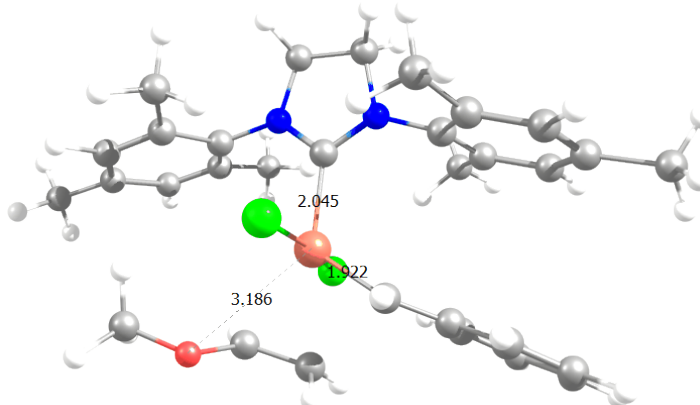
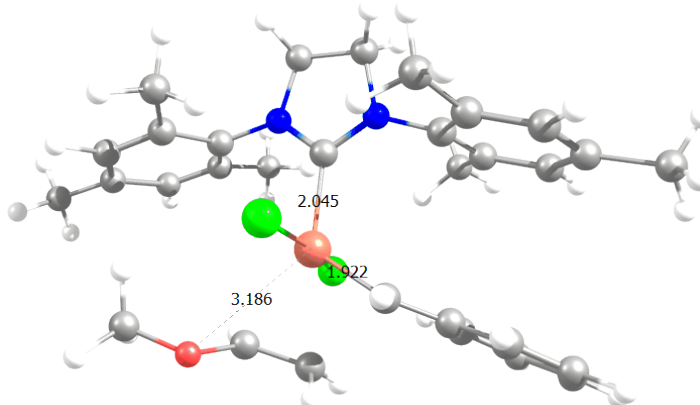
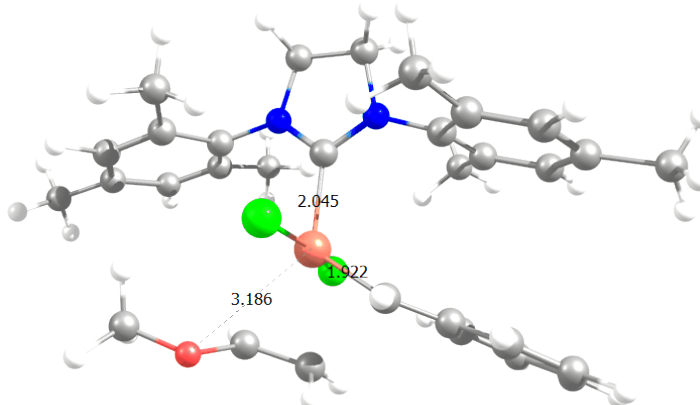
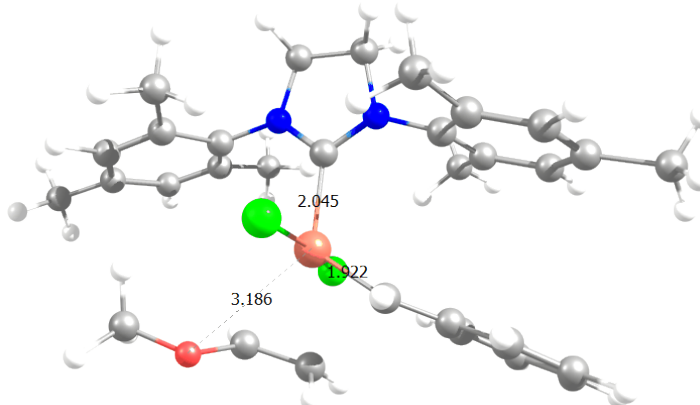
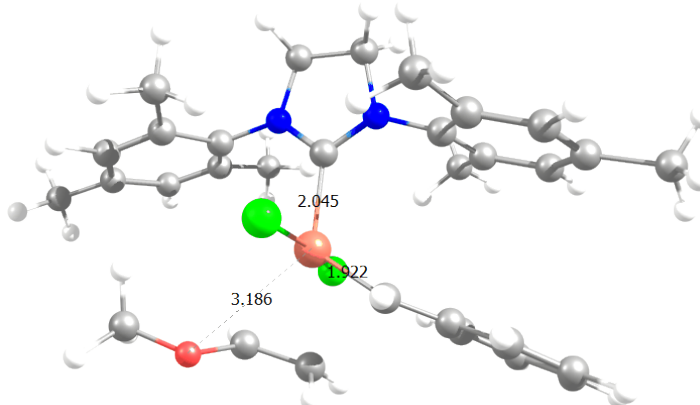
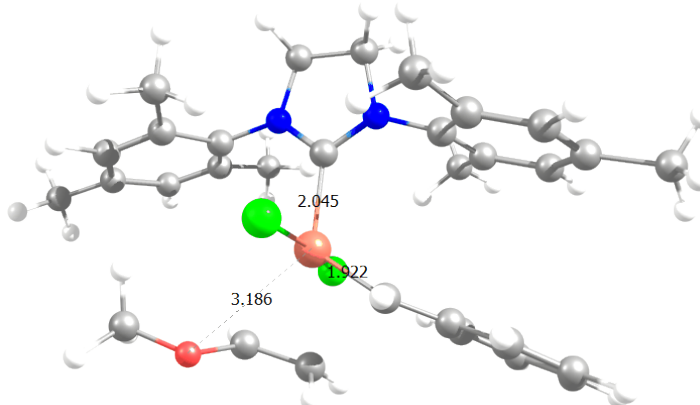
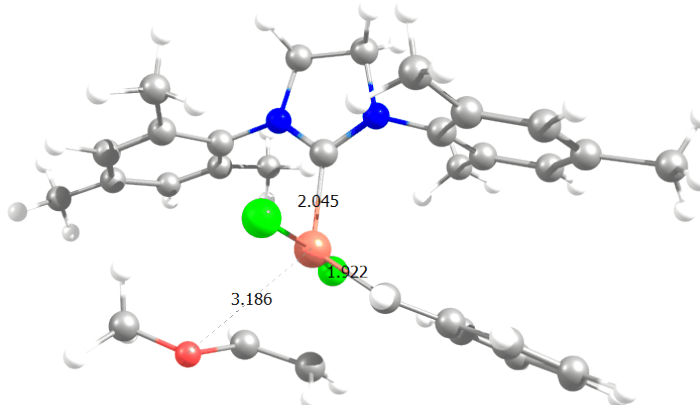
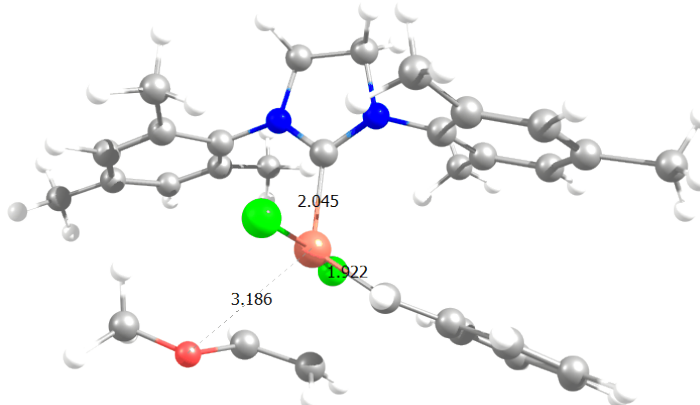
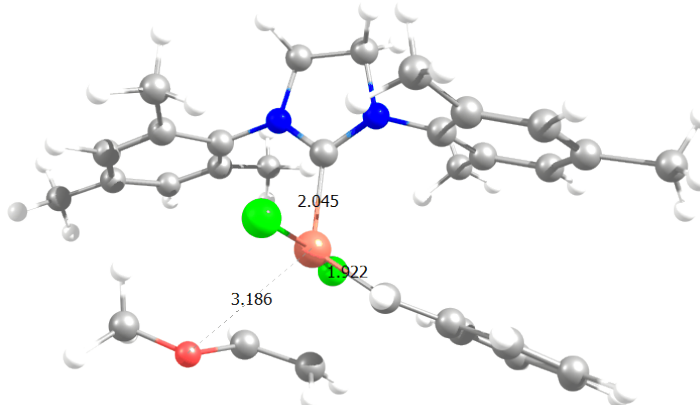
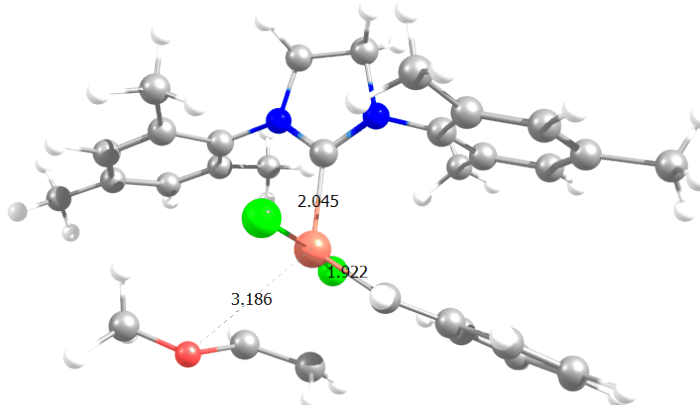
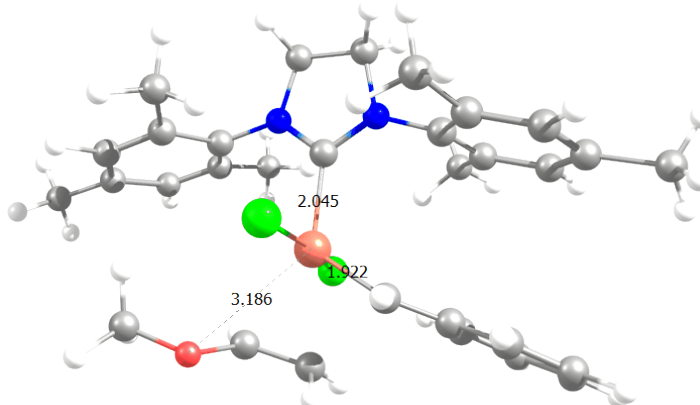
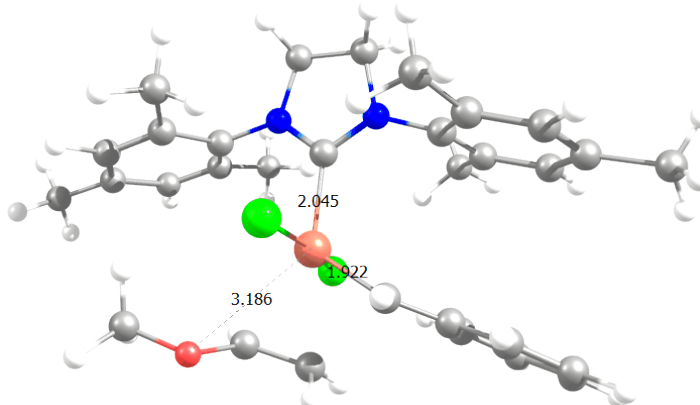
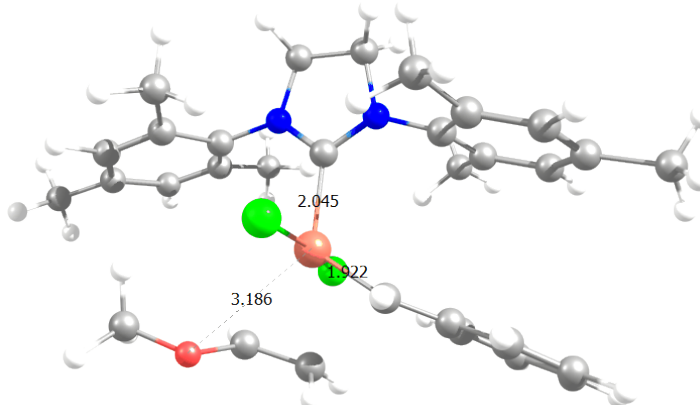
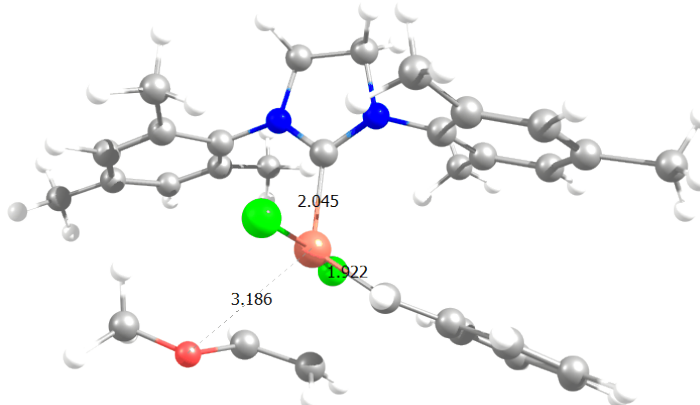
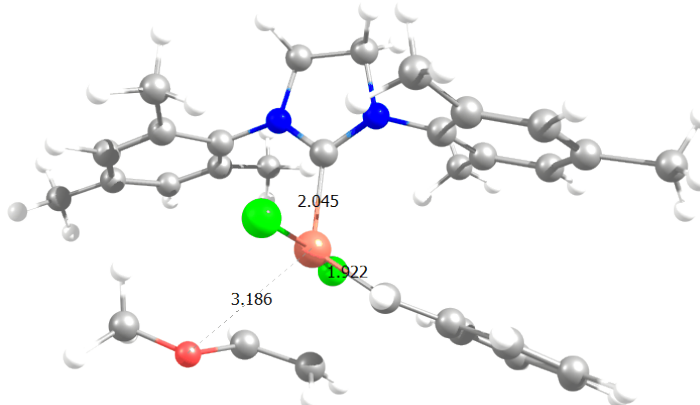
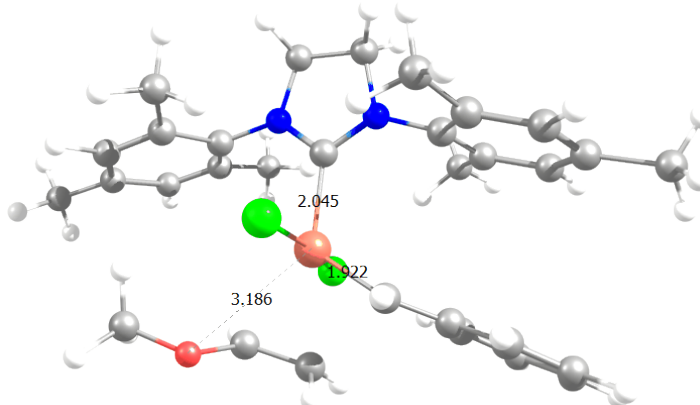
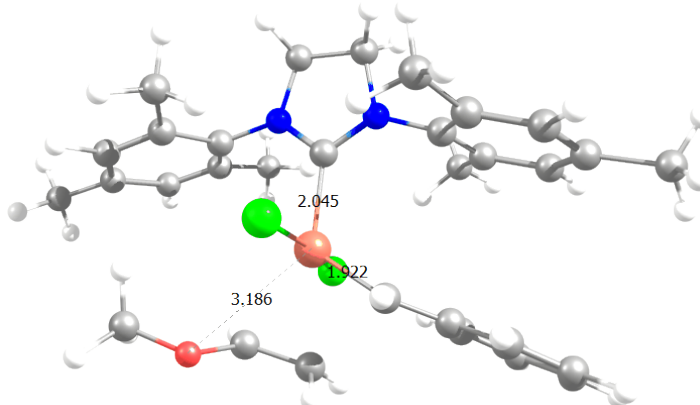
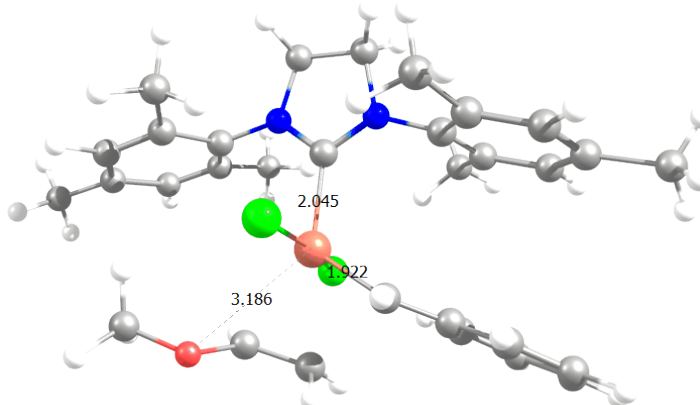
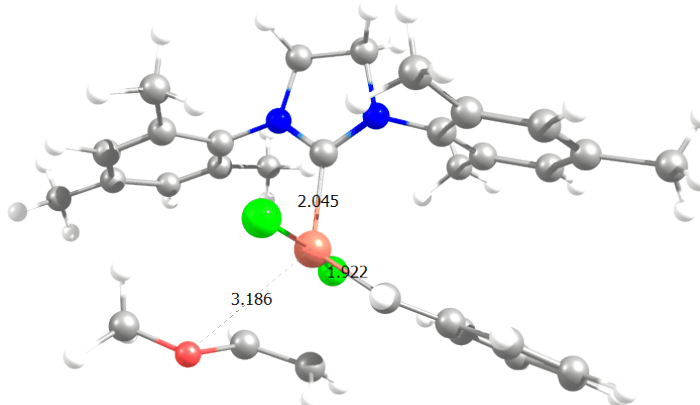
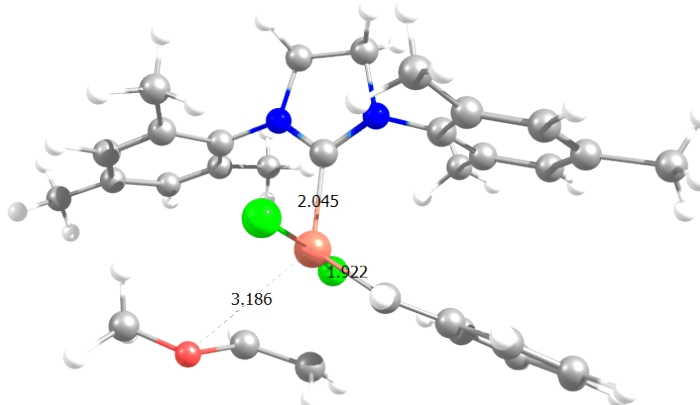
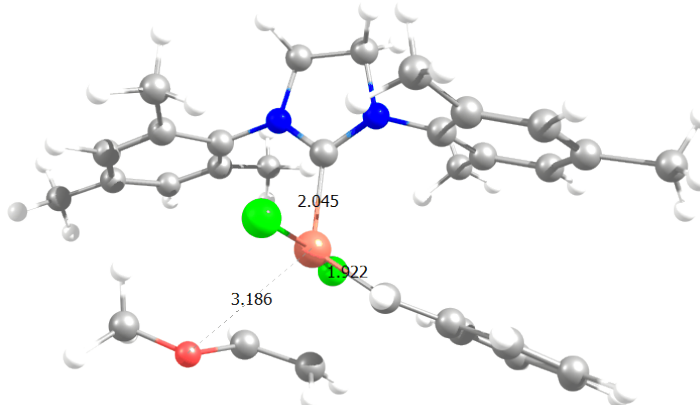
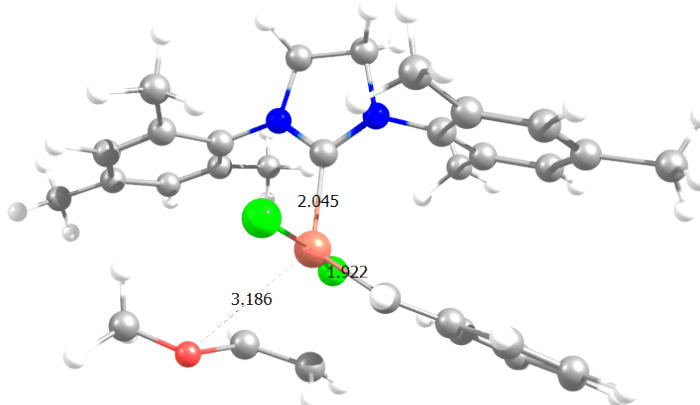
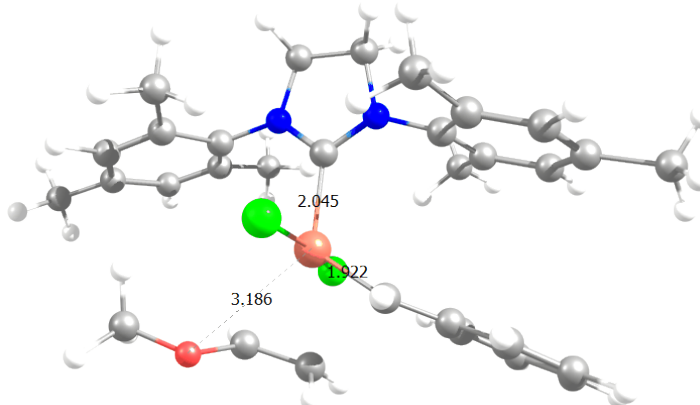
Rh-III-TZVP+					
		Rh	-0.501072	0.686328	-0.150898
		Cl	-0.472279	0.956285	2.183602
<p>Zero-point correction= 0.601183 (Hartree/Particle)            Thermal correction to Energy= 0.643813            Thermal correction to Enthalpy= 0.644758            Thermal correction to Gibbs Free Energy= 0.523083            Sum of electronic and Zero-point Energies= -2419.756824            Sum of electronic and thermal Energies= -2419.714193            Sum of electronic and thermal Enthalpies= -2419.713249            Sum of electronic and thermal Free Energies= -2419.834923</p>		Cl	-0.844058	0.488522	-2.500227
		N	-1.878393	-1.832519	0.272625
		N	0.277998	-2.296367	0.171101
		C	-0.646075	-1.321593	0.101697
<p>Zero-point correction= 0.601196 (Hartree/Particle)            Thermal correction to Energy= 0.642959            Thermal correction to Enthalpy= 0.643903            Thermal correction to Gibbs Free Energy= 0.524236            Sum of electronic and Zero-point Energies= -2419.745750            Sum of electronic and thermal Energies= -2419.703988            Sum of electronic and thermal Enthalpies= -2419.703044            Sum of electronic and thermal Free Energies= -2419.822711</p>		C	-1.856401	-3.305354	0.469193
		H	-2.415006	-3.795326	-0.341630
		H	-2.331699	-3.558771	1.427212
		C	-0.348474	-3.626255	0.441260
		H	0.022640	-4.018022	1.399057
		H	-0.074342	-4.333746	-0.353441
		C	-3.114892	-1.082175	0.233317
		C	-3.679015	-0.611097	1.444410
		C	-3.121575	-0.967656	2.799835
		H	-3.251389	-0.138409	3.508396
		H	-2.054304	-1.211932	2.771653
		H	-3.669483	-1.834264	3.208562
		C	-4.864209	0.132853	1.368351
		H	-5.297986	0.516821	2.295987
		C	-5.523727	0.366880	0.153614
		C	-6.780766	1.199249	0.101989
		H	-7.438600	0.885696	-0.720862
		H	-6.538790	2.262924	-0.059868
		H	-7.346068	1.133034	1.042245
		C	-4.989316	-0.206305	-1.009501
		H	-5.522383	-0.089076	-1.957301
		C	-3.806994	-0.957909	-0.996960
		C	-3.379705	-1.681857	-2.249561
		H	-3.592677	-1.079911	-3.142986
		H	-3.948062	-2.623133	-2.345927
		H	-2.310251	-1.918722	-2.260617
		C	1.707273	-2.215356	0.026177
		C	2.272254	-2.432372	-1.254005
		C	1.411309	-2.636652	-2.476306
		H	2.034595	-2.742792	-3.373969
Rh-III-IVTZVP+		Rh	0.304969	-0.792121	-0.210013
		Cl	0.431816	-1.220499	2.107874
		Cl	0.624635	-0.390246	-2.518737
		N	1.651357	1.835296	0.302740
		N	-0.528244	2.119016	0.075840
		C	0.471930	1.224198	0.088973
		C	1.487050	3.302402	0.503600
		H	2.114048	3.848908	-0.213829
		H	1.802657	3.570421	1.522712
		C	-0.020398	3.510128	0.266367
		H	-0.531666	3.975183	1.120400
		H	-0.234427	4.102911	-0.634445
		C	2.955998	1.219400	0.394814
		C	3.449946	0.825305	1.660281
		C	2.711762	1.096801	2.947887
		H	2.900307	0.302104	3.682337
		H	1.627043	1.168736	2.812295
		H	3.073089	2.040430	3.391788
		C	4.723075	0.238101	1.713770
		H	5.103535	-0.091932	2.684764
		C	5.530338	0.097044	0.577337
		C	6.914443	-0.496975	0.678193
		H	7.234065	-0.945954	-0.272927
		H	6.968763	-1.266216	1.461771
		H	7.652831	0.280435	0.935019
		C	5.039679	0.580871	-0.645058
		H	5.674769	0.528944	-1.534382
		C	3.771681	1.167243	-0.762679
		C	3.350333	1.784976	-2.072669
		H	4.010256	1.454655	-2.886219
		H	3.426660	2.884804	-2.025207
		H	2.319177	1.525091	-2.345072
		C	-1.947324	1.906014	-0.075928
		C	-2.540730	2.082889	-1.345268
		C	-1.731751	2.426653	-2.571553
		H	-2.328269	2.275312	-3.481259

Table S1. Cont.

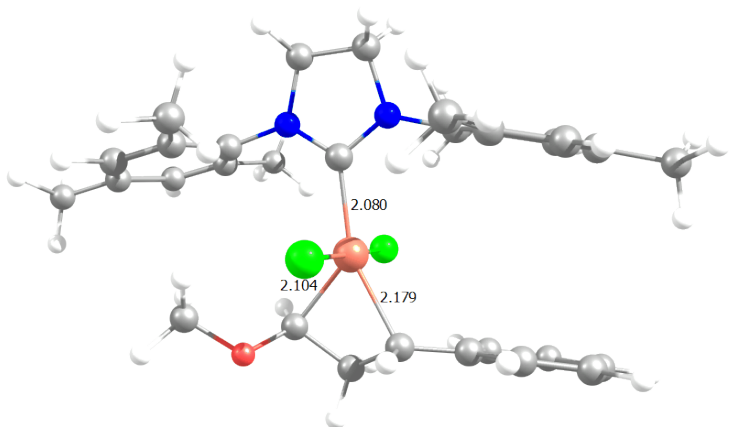
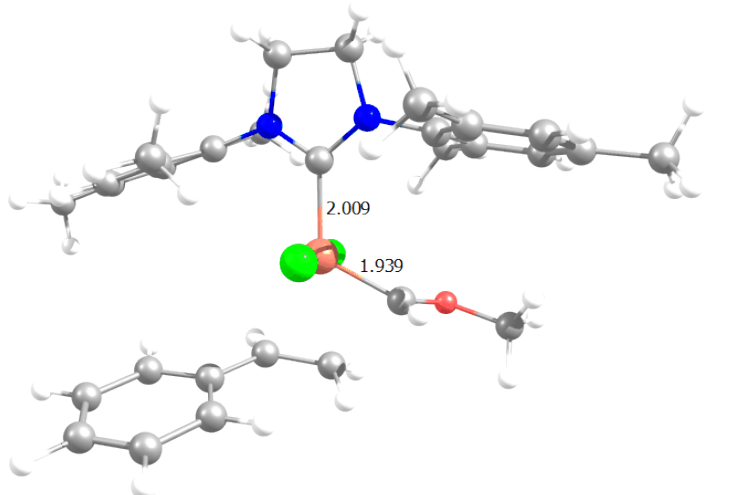
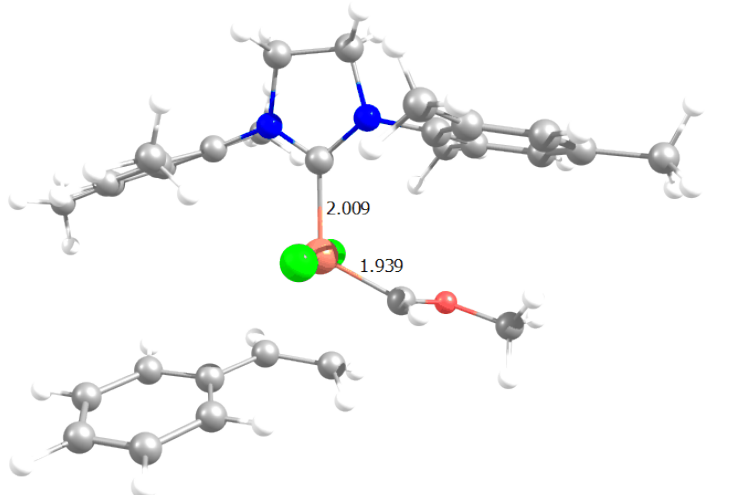
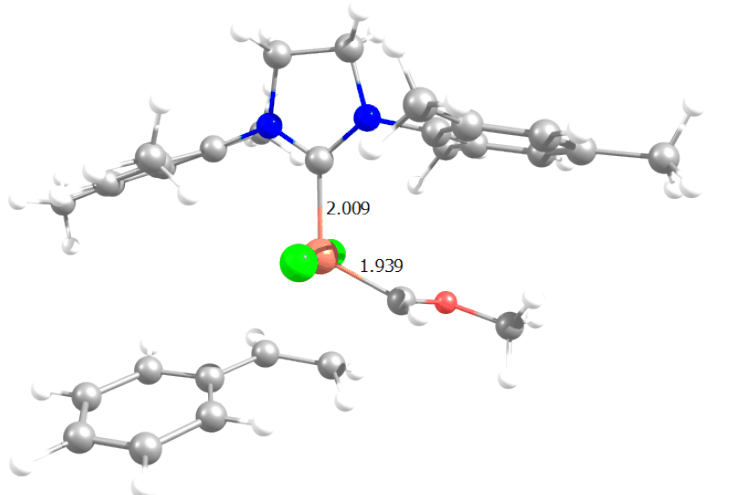
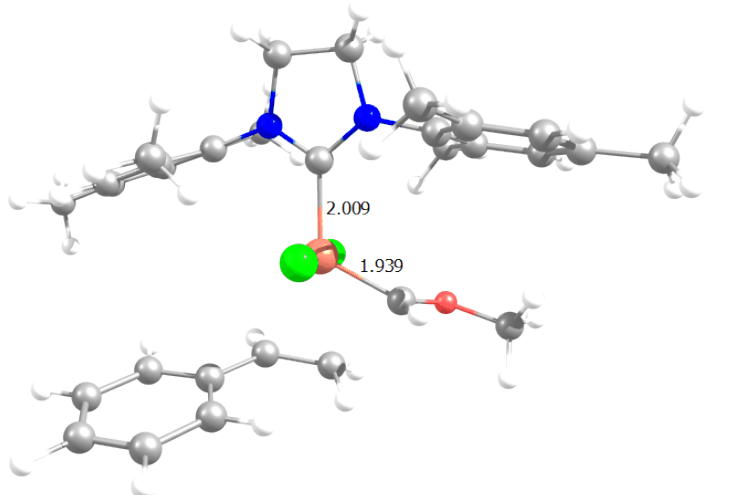
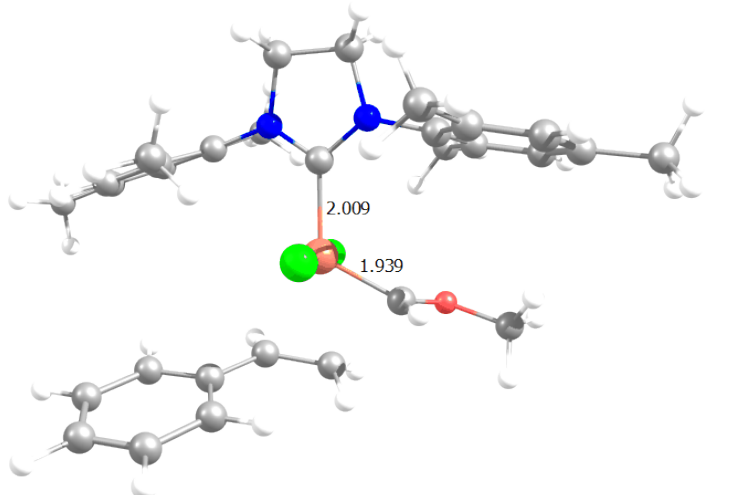
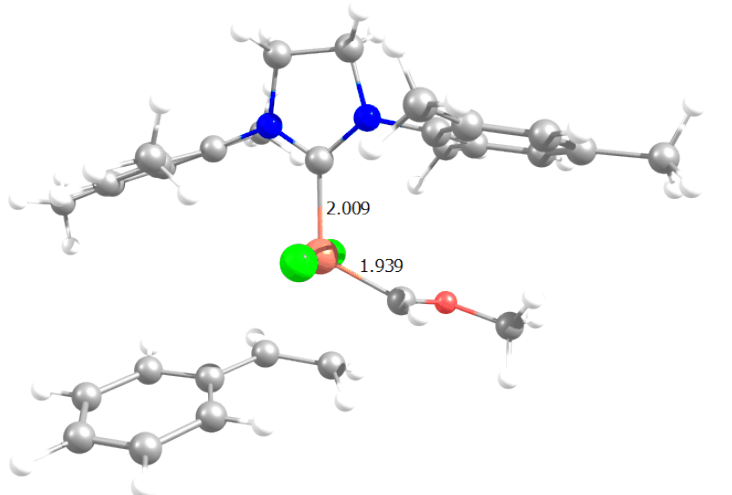
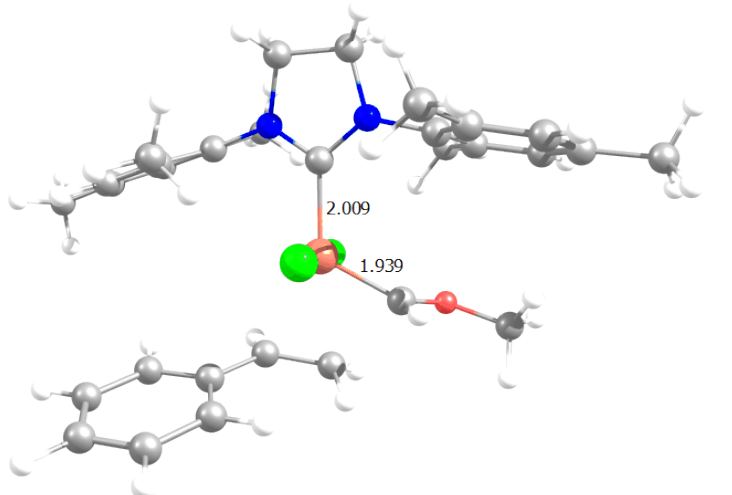
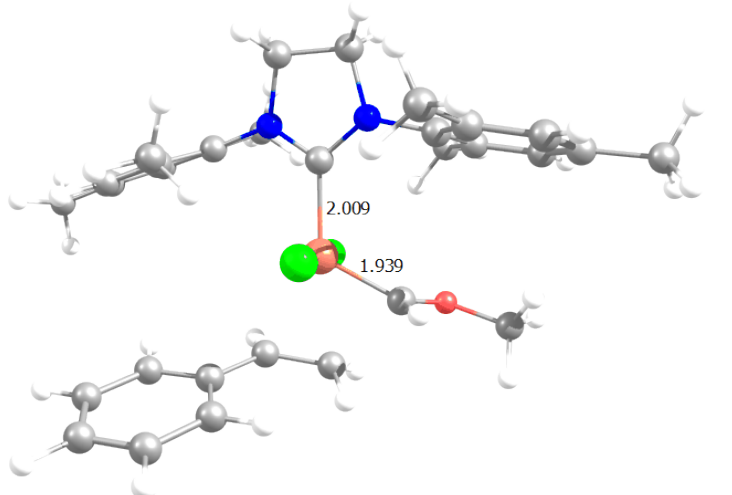
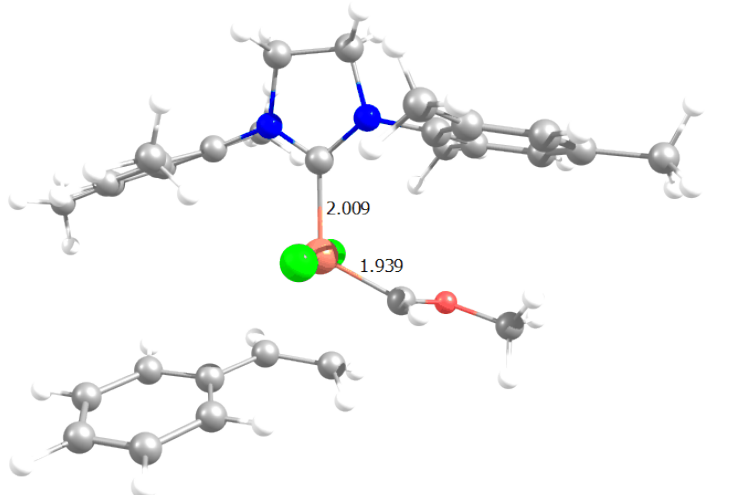
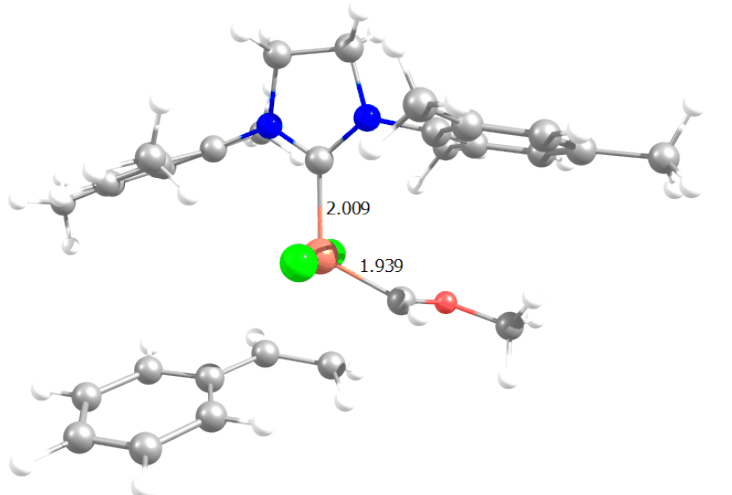
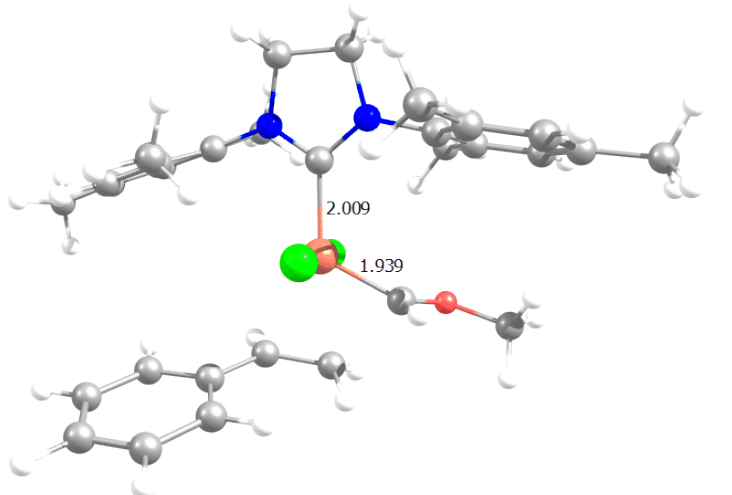
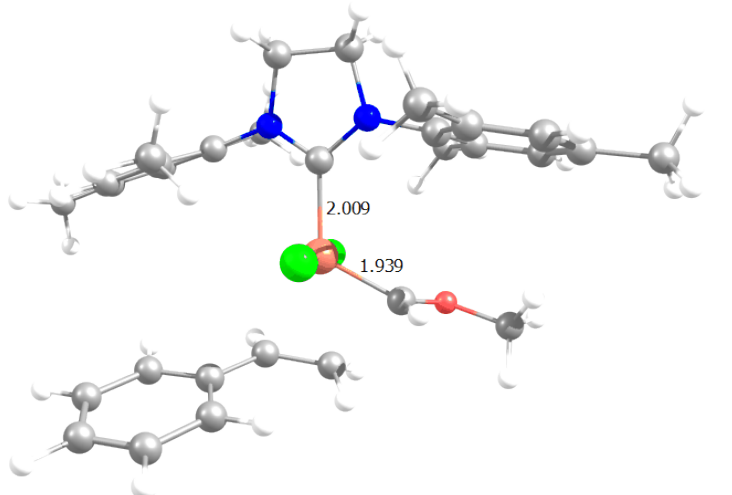
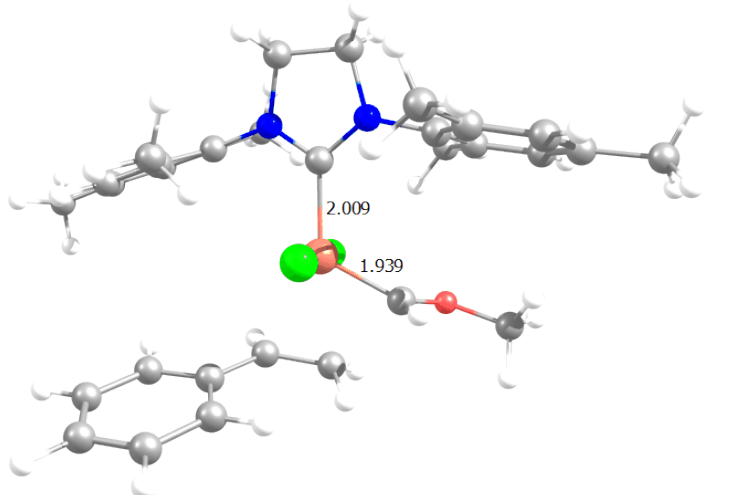
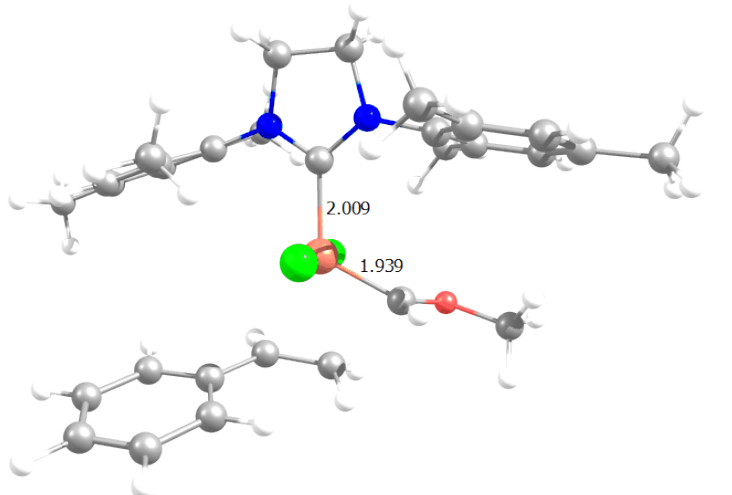
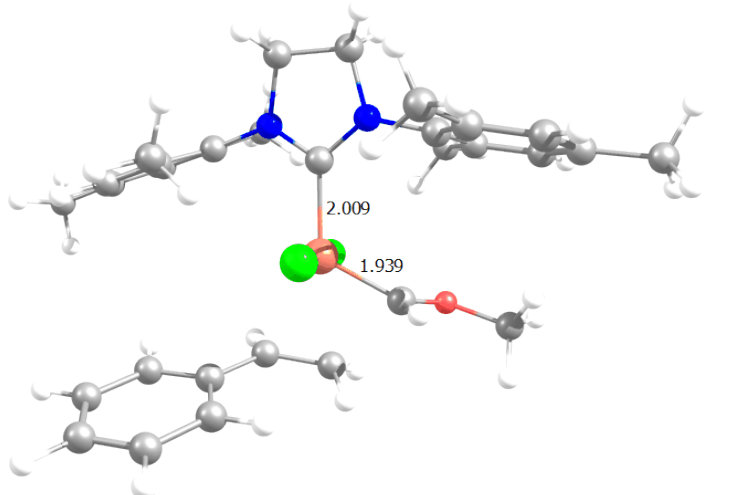
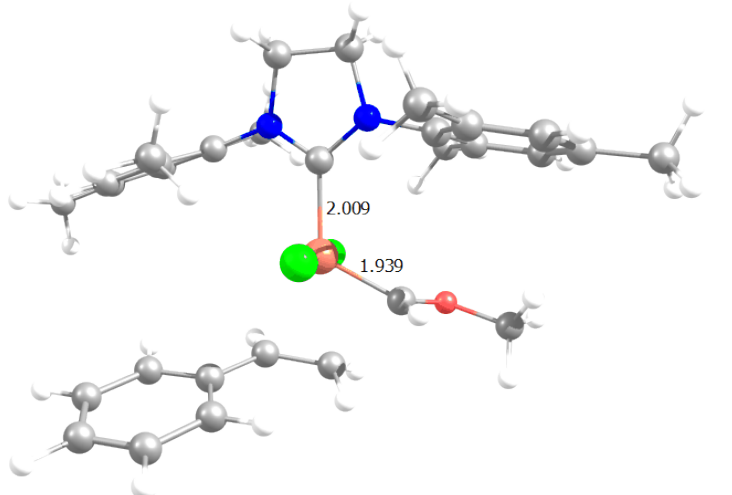
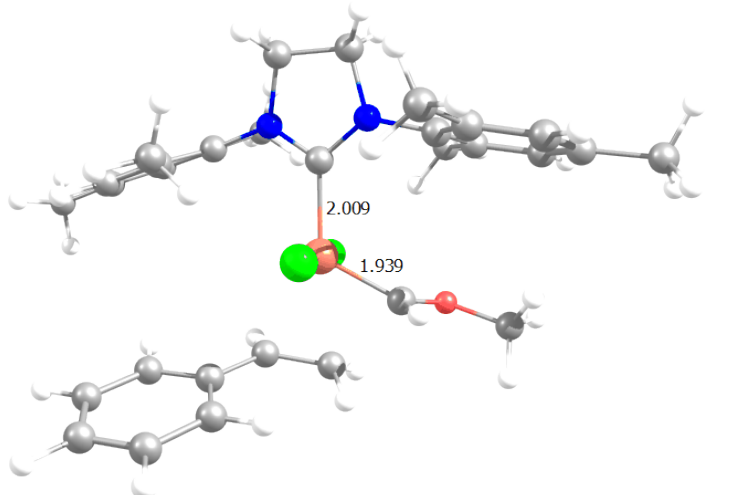
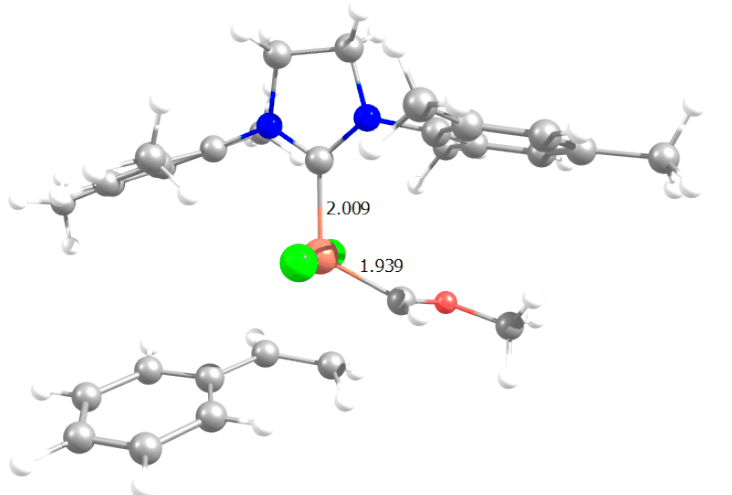
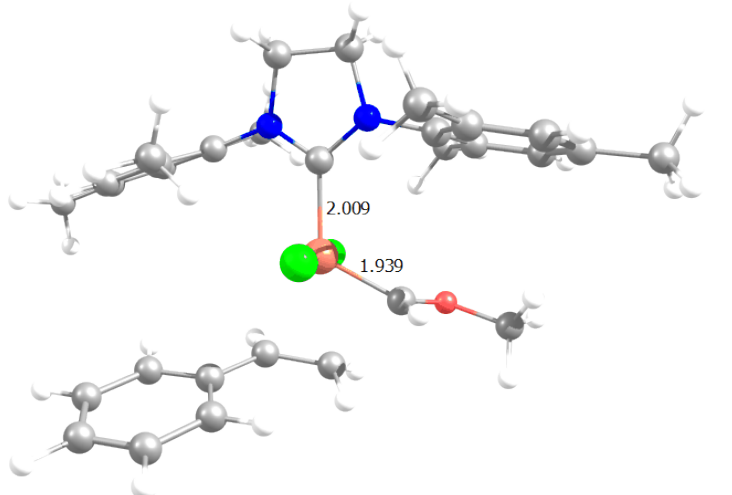
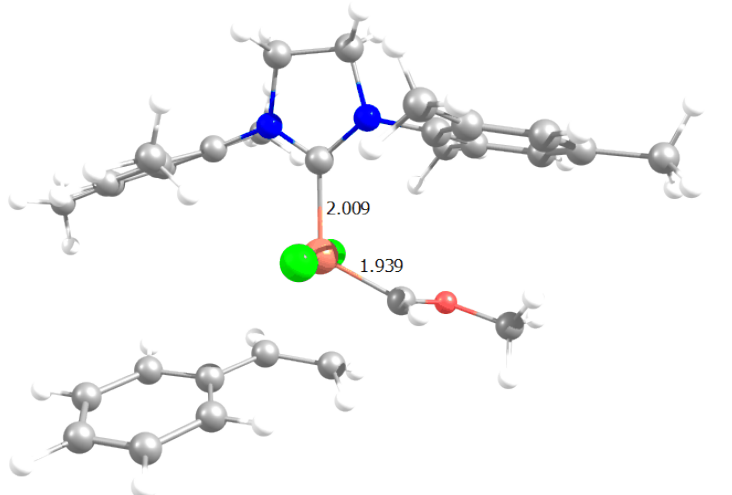
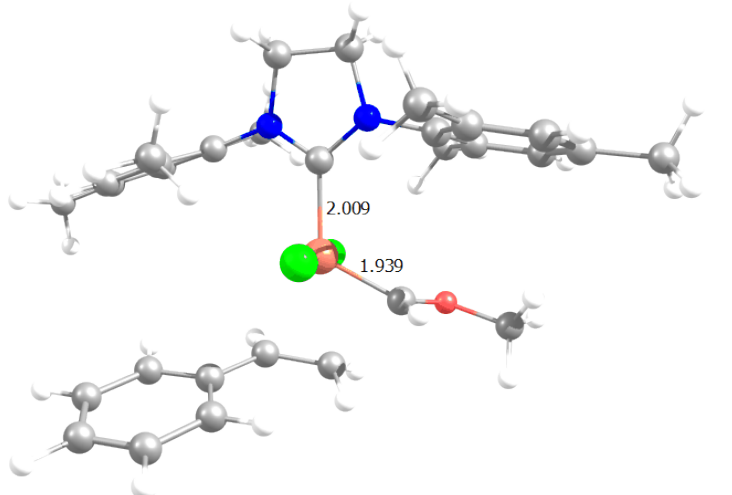
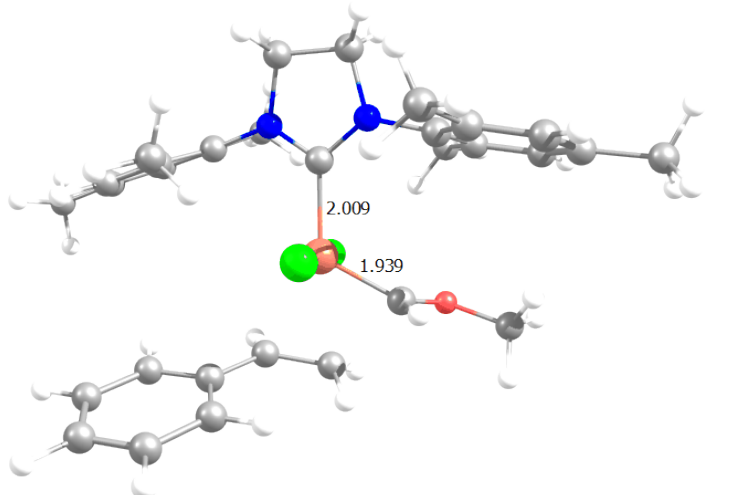
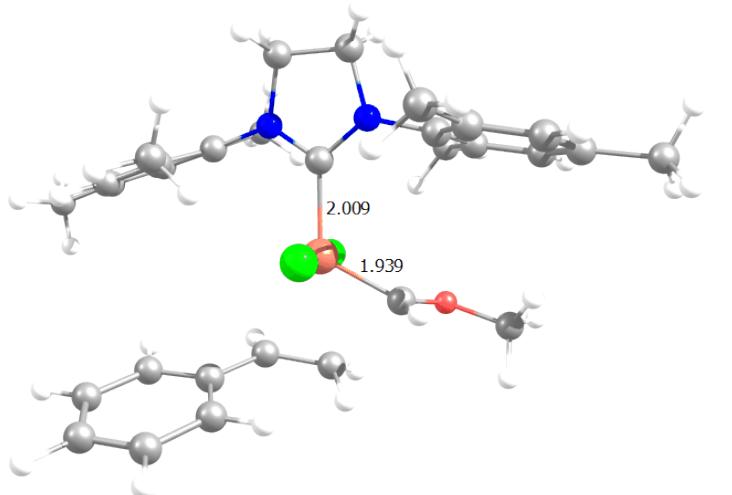
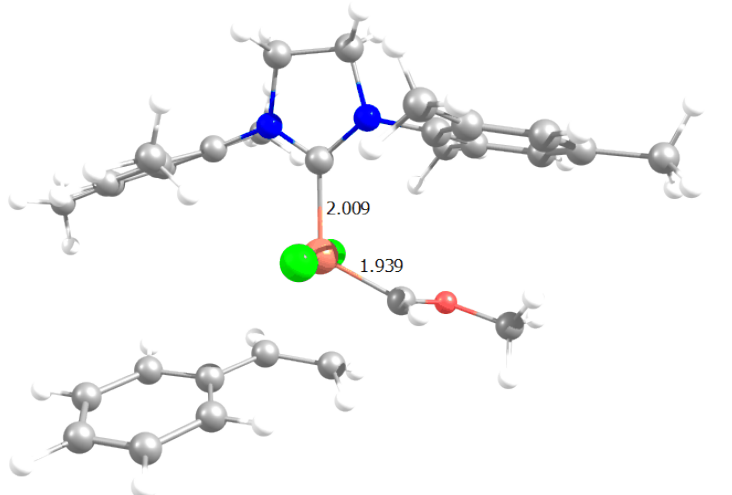
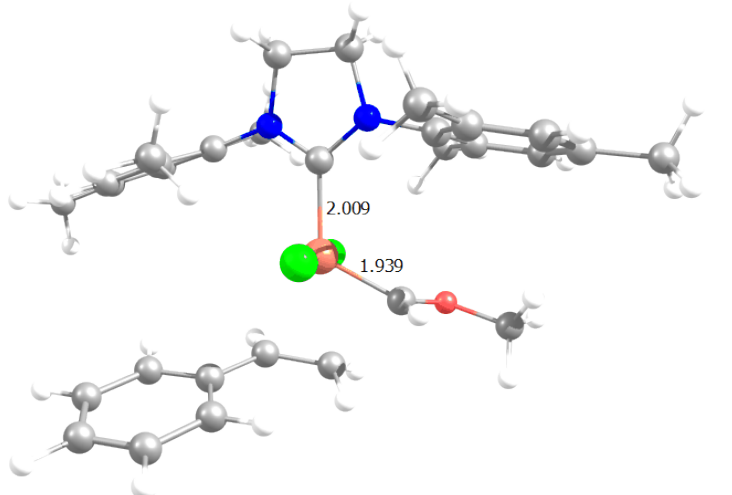
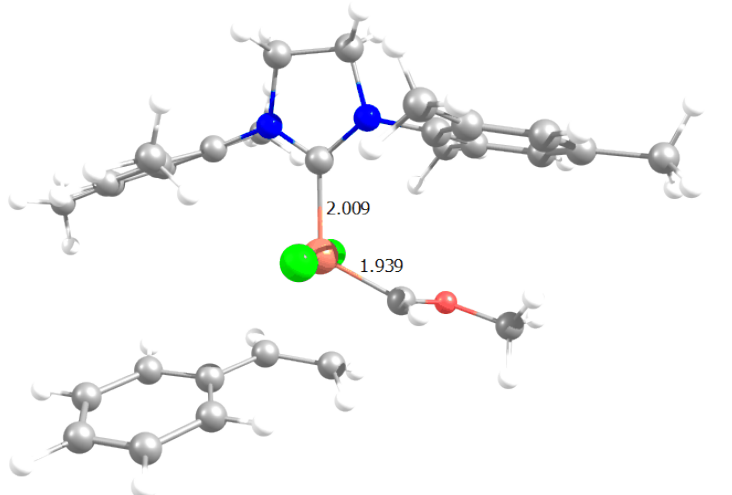
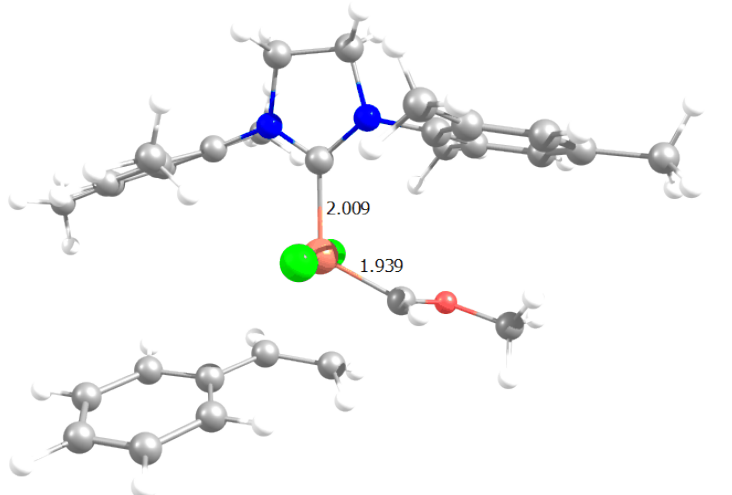
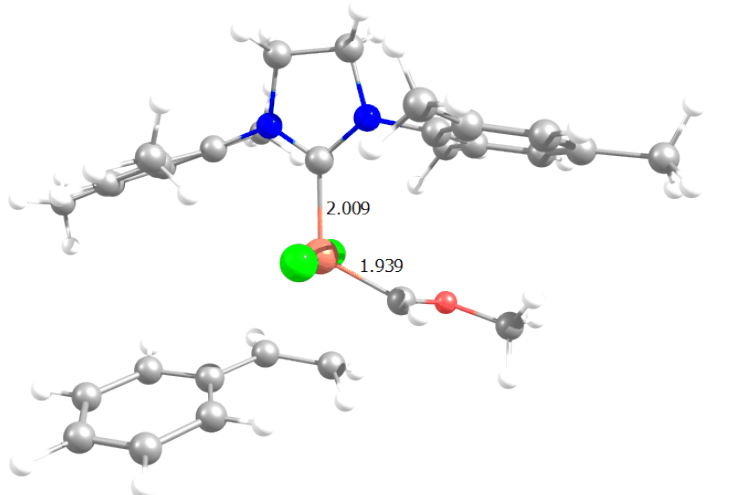
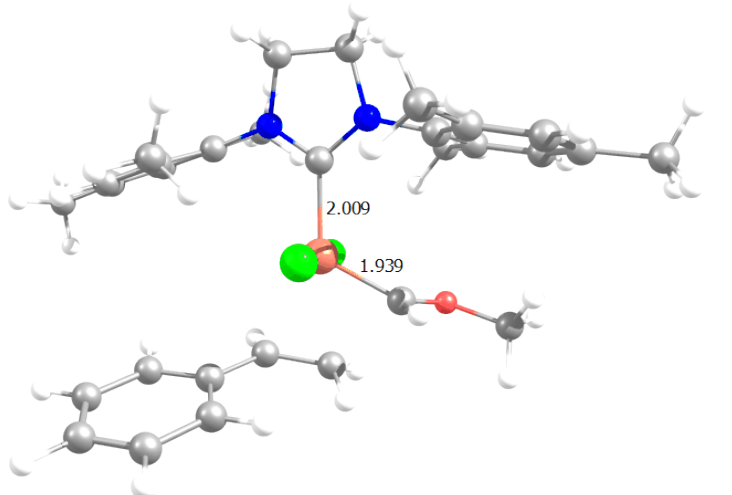
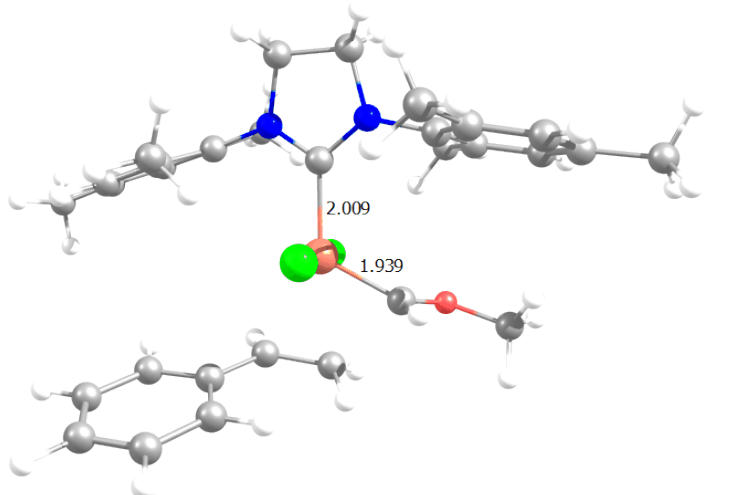
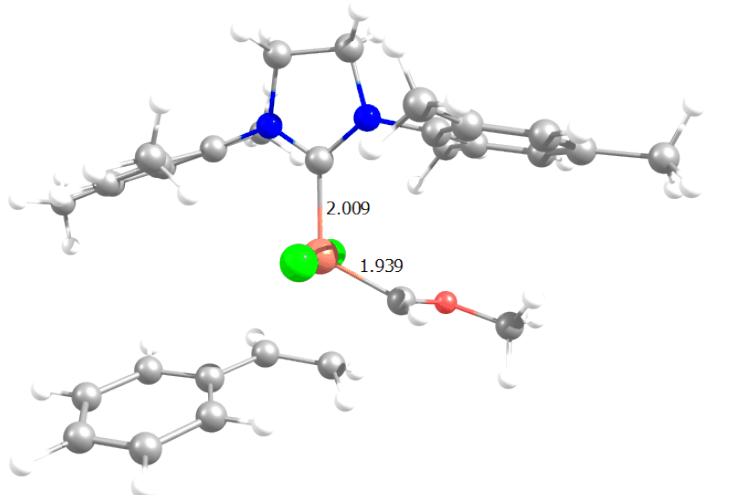
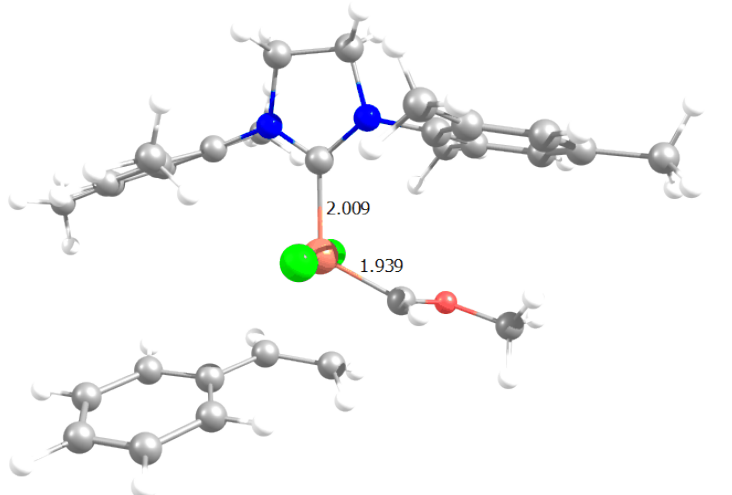
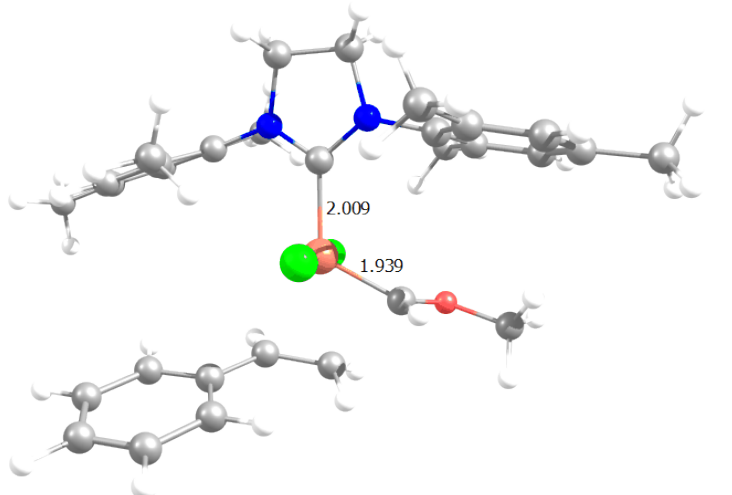
Rh-IVTZVPd					
		Rh	0.062627	-0.782367	-0.097343
		Cl	-0.349262	-0.854818	2.263451
<p>Zero-point correction= 0.600264 (Hartree/Particle)            Thermal correction to Energy= 0.642308            Thermal correction to Enthalpy= 0.643252            Thermal correction to Gibbs Free Energy= 0.521865            Sum of electronic and Zero-point Energies= -2419.964927            Sum of electronic and thermal Energies= -2419.922884            Sum of electronic and thermal Enthalpies= -2419.921940            Sum of electronic and thermal Free Energies= -2420.043327</p>		Cl	0.501689	-0.661381	-2.442868
		N	1.903076	1.720336	0.125901
		N	-0.232898	2.226434	0.004572
		C	0.655419	1.207239	0.035450
<p>Zero-point correction= 0.597734 (Hartree/Particle)            Thermal correction to Energy= 0.639853            Thermal correction to Enthalpy= 0.640798            Thermal correction to Gibbs Free Energy= 0.519430            Sum of electronic and Zero-point Energies= -2419.943444            Sum of electronic and thermal Energies= -2419.901325            Sum of electronic and thermal Enthalpies= -2419.900381            Sum of electronic and thermal Free Energies= -2420.021748</p>		C	1.894347	3.203392	0.272446
		H	2.600405	3.658521	-0.435640
		H	2.202979	3.475440	1.295076
		C	0.432110	3.557137	-0.022414
		H	-0.014430	4.218825	0.732308
		H	0.298697	4.018317	-1.014129
		C	3.166722	1.033848	0.207038
		C	3.652008	0.610416	1.464141
		C	2.849813	0.788506	2.727849
		H	3.402318	0.394562	3.592094
		H	1.875807	0.275477	2.676380
		H	2.643322	1.853344	2.926035
		C	4.930875	0.035187	1.516756
		H	5.311427	-0.300680	2.486099
		C	5.739226	-0.093592	0.378852
		C	7.105181	-0.732995	0.465952
		H	7.773986	-0.361606	-0.324019
		H	7.038254	-1.827927	0.351038
		H	7.579848	-0.536911	1.438634
		C	5.239716	0.377534	-0.842831
		H	5.861661	0.305906	-1.740157
		C	3.964409	0.950839	-0.955419
		C	3.472530	1.453209	-2.289612
		H	4.210892	1.243431	-3.075865
		H	3.303516	2.542866	-2.279297
		H	2.519438	0.973900	-2.565837
		C	-1.675911	2.160866	-0.049349
		C	-2.330965	2.163938	-1.300757
		C	-1.575268	2.201702	-2.604292
		H	-2.276073	2.208577	-3.450669
Rh-IV-VTZVPd		Rh	-0.024494	0.551432	-0.484500
		Cl	-0.027329	1.658528	1.634658
		Cl	0.128450	-0.530013	-2.601832
		N	-1.741580	-1.500234	0.941013
		N	0.351802	-2.151854	0.730981
		C	-0.526176	-1.160495	0.439696
		C	-1.741628	-2.855105	1.551556
		H	-2.336538	-3.542654	0.927866
		H	-2.190793	-2.823426	2.554059
		C	-0.249213	-3.214981	1.574606
		H	0.181800	-3.170628	2.587845
		H	-0.037183	-4.206851	1.151627
		C	-3.011855	-0.855527	0.727477
		C	-3.596148	-0.127367	1.787684
		C	-2.880778	0.074592	3.098799
		H	-3.469913	0.721335	3.763754
		H	-1.893674	0.536359	2.940634
		H	-2.720900	-0.881102	3.625667
		C	-4.877074	0.411085	1.593187
		H	-5.329782	0.987657	2.405502
		C	-5.594757	0.215444	0.405181
		C	-6.995357	0.761475	0.247206
		H	-7.739984	0.062850	0.664265
		H	-7.251713	0.916935	-0.810975
		H	-7.117626	1.718647	0.775621
		C	-4.993957	-0.536386	-0.613499
		H	-5.542424	-0.714114	-1.543708
		C	-3.712202	-1.091701	-0.476331
		C	-3.120104	-1.910632	-1.593760
		H	-3.866648	-2.082629	-2.381636
		H	-2.774695	-2.895230	-1.240150
		H	-2.247410	-1.411222	-2.046445
		C	1.754554	-2.224011	0.396981
		C	2.140620	-3.019292	-0.706401
		C	1.126992	-3.734638	-1.562621
		H	1.624332	-4.249449	-2.396173

Table S1. Cont.

Rh-IVTZVP+					
		Rh	0.186384	-0.755017	-0.306649
<p>Zero-point correction= 0.602340 (Hartree/Particle)</p> <p>Thermal correction to Energy= 0.644487</p> <p>Thermal correction to Enthalpy= 0.645431</p> <p>Thermal correction to Gibbs Free Energy= 0.524178</p> <p>Sum of electronic and Zero-point Energies= -2419.753853</p> <p>Sum of electronic and thermal Energies= -2419.711706</p> <p>Sum of electronic and thermal Enthalpies= -2419.710762</p> <p>Sum of electronic and thermal Free Energies= -2419.832015</p>		Cl	0.116116	-1.354143	1.984454
		Cl	0.382833	-0.124721	-2.574171
		N	1.729373	1.694894	0.487524
		N	-0.440976	2.106046	0.322455
		C	0.521345	1.179022	0.206632
		C	1.613074	3.113503	0.937635
		H	2.316269	3.739570	0.373069
		H	1.864167	3.174948	2.007100
		C	0.139993	3.442522	0.648481
		H	-0.385811	3.872119	1.511069
		H	0.012340	4.113134	-0.214095
		C	3.030664	1.063966	0.455432
		C	3.576364	0.536204	1.646628
		C	2.860185	0.597962	2.972983
		H	3.195421	-0.213567	3.633134
		H	1.771563	0.516360	2.873590
		H	3.095540	1.545400	3.487974
		C	4.879409	0.013567	1.595427
		H	5.306449	-0.406099	2.510659
		C	5.659913	0.058498	0.434134
		C	7.063411	-0.496397	0.412636
		H	7.760576	0.201043	-0.075159
		H	7.109997	-1.442769	-0.150956
		H	7.433074	-0.696023	1.427504
		C	5.104723	0.653530	-0.711249
		H	5.712403	0.743463	-1.616348
		C	3.805914	1.179511	-0.725034
		C	3.295374	1.892739	-1.951571
		H	4.033395	1.838338	-2.762642
		H	3.115481	2.961285	-1.746452
		H	2.351569	1.462343	-2.315956
		C	-1.870072	1.986510	0.120608
		C	-2.422656	2.344846	-1.129974
		C	-1.578695	2.819393	-2.286589
		H	-2.132296	2.727637	-3.230783
Rh-IV-VTZVP+					
		Rh	-0.075444	0.637927	-0.425723
<p>Zero-point correction= 0.601210 (Hartree/Particle)</p> <p>Thermal correction to Energy= 0.643130</p> <p>Thermal correction to Enthalpy= 0.644074</p> <p>Thermal correction to Gibbs Free Energy= 0.523145</p> <p>Sum of electronic and Zero-point Energies= -2419.751056</p> <p>Sum of electronic and thermal Energies= -2419.709136</p> <p>Sum of electronic and thermal Enthalpies= -2419.708192</p> <p>Sum of electronic and thermal Free Energies= -2419.829121</p>		Cl	-0.081072	1.530051	1.773219
		Cl	0.012446	-0.292731	-2.590203
		N	-1.737569	-1.624895	0.725583
		N	0.407618	-2.143665	0.587575
		C	-0.519125	-1.202222	0.351241
		C	-1.683472	-3.002149	1.300113
		H	-2.344336	-3.666328	0.725559
		H	-2.032228	-2.976963	2.341936
		C	-0.193670	-3.374032	1.175996
		H	0.278689	-3.589274	2.144502
		H	-0.018162	-4.224735	0.502508
		C	-3.015198	-0.960714	0.607266
		C	-3.570283	-0.327541	1.741853
		C	-2.863236	-0.289755	3.073793
		H	-3.255273	0.525718	3.696416
		H	-1.781602	-0.140739	2.964917
		H	-3.032566	-1.226740	3.631961
		C	-4.850113	0.234650	1.618530
		H	-5.283503	0.737761	2.487779
		C	-5.599763	0.136370	0.437721
		C	-7.001361	0.692826	0.362466
		H	-7.729079	-0.034931	0.757726
		H	-7.295533	0.916366	-0.672774
		H	-7.105790	1.610082	0.959951
		C	-5.028728	-0.536990	-0.652352
		H	-5.606481	-0.648828	-1.574470
		C	-3.747774	-1.105716	-0.592824
		C	-3.203511	-1.866426	-1.775333
		H	-3.944843	-1.899936	-2.584586
		H	-2.960624	-2.908459	-1.510693
		H	-2.284307	-1.408812	-2.172260
		C	1.822294	-2.091976	0.290461
		C	2.292663	-2.676248	-0.909894
		C	1.380350	-3.375299	-1.887264
		H	1.815432	-3.366297	-2.895626

Table S1. Cont.

Rh-VTZVPd					
		Rh	0.208588	-0.796872	-0.549303
		Cl	0.100536	-1.851202	1.603836
<p>Zero-point correction= 0.597816 (Hartree/Particle)            Thermal correction to Energy= 0.640667            Thermal correction to Enthalpy= 0.641611            Thermal correction to Gibbs Free Energy= 0.519293            Sum of electronic and Zero-point Energies= -2419.954073            Sum of electronic and thermal Energies= -2419.911222            Sum of electronic and thermal Enthalpies= -2419.910278            Sum of electronic and thermal Free Energies= -2420.032596</p>		Cl	0.203380	0.181379	-2.726942
		N	1.772627	1.549319	0.775911
<p>Rh-V-VITZVPd</p>		N	-0.340313	2.075163	0.543238
		C	0.573128	1.101119	0.325662
<p>Zero-point correction= 0.596425 (Hartree/Particle)            Thermal correction to Energy= 0.639874            Thermal correction to Enthalpy= 0.640818            Thermal correction to Gibbs Free Energy= 0.512995            Sum of electronic and Zero-point Energies= -2419.947654            Sum of electronic and thermal Energies= -2419.904205            Sum of electronic and thermal Enthalpies= -2419.903261            Sum of electronic and thermal Free Energies= -2420.031084</p>		C	1.721334	2.950166	1.276358
		H	2.292085	3.608189	0.600868
<p>Rh</p>		H	2.169203	3.014317	2.278350
		C	0.218246	3.250344	1.267056
<p>Cl</p>		H	-0.213926	3.299662	2.279517
		H	-0.035103	4.180136	0.738211
<p>C</p>		C	3.062596	0.918839	0.699594
		C	3.569986	0.265308	1.844799
<p>C</p>		C	2.743231	0.115501	3.095992
		H	3.305688	-0.428985	3.867033
<p>H</p>		H	1.810459	-0.433561	2.888383
		H	2.463029	1.094911	3.517607
<p>C</p>		C	4.873577	-0.250535	1.789322
		H	5.269298	-0.766877	2.669171
<p>C</p>		C	5.684293	-0.105323	0.654872
		C	7.104690	-0.621129	0.647533
<p>H</p>		H	7.794636	0.119896	1.084978
		H	7.455040	-0.828098	-0.374247
<p>H</p>		H	7.202066	-1.543590	1.238960
		C	5.154166	0.567165	-0.455104
<p>H</p>		H	5.775145	0.704891	-1.346026
		C	3.853688	1.096522	-0.457042
<p>C</p>		C	3.330174	1.826079	-1.667277
		H	4.089207	1.850035	-2.461464
<p>H</p>		H	3.066745	2.870053	-1.430386
		H	2.421392	1.348178	-2.069568
<p>C</p>		C	-1.757421	2.063540	0.275600
		C	-2.232523	2.726145	-0.878250
<p>C</p>		C	-1.292148	3.330884	-1.889779
		H	-1.857960	3.806360	-2.702950
<p>Rh</p>		Rh	0.289028	-0.529290	-0.546118
		Cl	-0.293921	-1.676219	1.462607
<p>Cl</p>		Cl	0.311451	0.298799	-2.740632
		N	2.295203	1.302534	0.848576
<p>N</p>		N	0.307182	2.227129	0.693368
		C	1.034421	1.126431	0.390943
<p>C</p>		C	2.500650	2.646341	1.452917
		H	3.186030	3.237786	0.823992
<p>H</p>		H	2.948543	2.549392	2.452368
		C	1.076254	3.223652	1.485333
<p>H</p>		H	0.667297	3.286119	2.506236
		H	1.002439	4.217186	1.020981
<p>C</p>		C	3.429258	0.430772	0.704003
		C	3.776392	-0.416157	1.778603
<p>C</p>		C	2.901264	-0.530825	3.000515
		H	3.353745	-1.207146	3.738823
<p>H</p>		H	1.903224	-0.918796	2.735446
		H	2.748316	0.444899	3.489371
<p>C</p>		C	4.952573	-1.172961	1.669115
		H	5.227676	-1.835552	2.495193
<p>C</p>		C	5.788208	-1.089127	0.545669
		C	7.083397	-1.865371	0.483285
<p>H</p>		H	7.903137	-1.300259	0.957752
		H	7.385209	-2.065985	-0.555123
<p>H</p>		H	7.004806	-2.827276	1.011265
		C	5.404424	-0.243263	-0.504632
<p>H</p>		H	6.037253	-0.171694	-1.394493
		C	4.232914	0.527203	-0.451889
<p>C</p>		C	3.836486	1.397857	-1.616878
		H	4.625975	1.403030	-2.380886
<p>H</p>		H	3.656749	2.441116	-1.312531
		H	2.906074	1.032972	-2.083623
<p>C</p>		C	-1.081731	2.463662	0.382748
		C	-1.399660	3.184275	-0.789932
<p>C</p>		C	-0.332479	3.659458	-1.742383
		H	-0.775042	4.271499	-2.540417

Table S1. Cont.

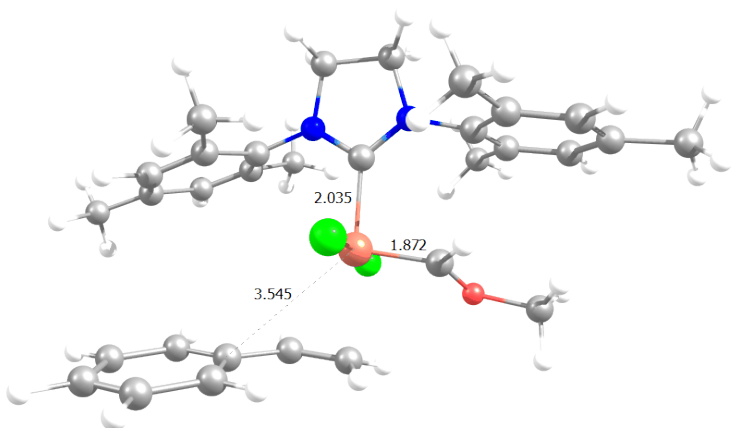
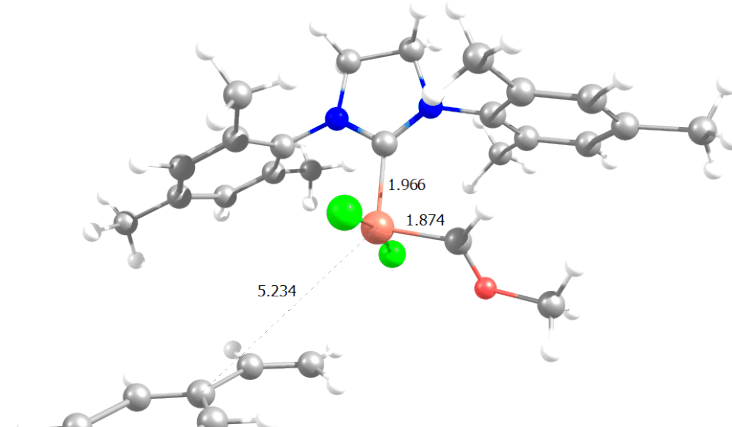
Rh-VTZVP+					
		Rh	0.033553	-0.667475	-0.419953
		Cl	-0.218722	-1.511013	1.776479
		Cl	0.062046	0.128009	-2.633074
		N	1.951867	1.496349	0.661502
		N	-0.163235	2.103679	0.533022
		C	0.711338	1.108179	0.307799
		C	1.973796	2.913313	1.132121
		H	2.561784	3.523321	0.430293
		H	2.445663	2.970995	2.122174
		C	0.482578	3.292546	1.152094
		H	0.089971	3.433469	2.170092
		H	0.258217	4.189861	0.559688
		C	3.200134	0.790780	0.543846
		C	3.728313	0.144567	1.688005
		C	2.964509	0.079045	2.986952
		H	3.500904	-0.539274	3.718587
		H	1.955544	-0.341031	2.851957
		H	2.843299	1.080132	3.432565
		C	5.001819	-0.433372	1.586198
		H	5.417501	-0.939534	2.462079
		C	5.770948	-0.346341	0.414560
		C	7.167401	-0.915569	0.363455
		H	7.893822	-0.190502	0.766185
		H	7.475900	-1.146538	-0.665793
		H	7.255740	-1.829657	0.968100
		C	5.221196	0.320626	-0.690624
		H	5.811259	0.413469	-1.607036
		C	3.947473	0.908374	-0.652336
		C	3.415352	1.648304	-1.853511
		H	4.131336	1.600902	-2.684494
		H	3.246178	2.714195	-1.629823
		H	2.455860	1.234570	-2.202429
		C	-1.586522	2.087821	0.277414
		C	-2.063462	2.646226	-0.936548
		C	-1.143418	3.278213	-1.950761
		H	-1.631368	3.334340	-2.932919
Zero-point correction= 0.600875 (Hartree/Particle) Thermal correction to Energy= 0.643807 Thermal correction to Enthalpy= 0.644751 Thermal correction to Gibbs Free Energy= 0.521724 Sum of electronic and Zero-point Energies= -2419.764427 Sum of electronic and thermal Energies= -2419.721496 Sum of electronic and thermal Enthalpies= -2419.720551 Sum of electronic and thermal Free Energies= -2419.843578					
Rh-V-VTZVP+					
		Rh	0.200440	-0.335712	-0.418595
		Cl	-0.455126	-1.152066	1.673355
		Cl	0.441273	0.295951	-2.636572
		N	2.574783	1.284717	0.563369
		N	0.606352	2.300882	0.535261
		C	1.264230	1.156496	0.293198
		C	2.876693	2.647231	1.097837
		H	3.679214	3.107032	0.505799
		H	3.214619	2.565400	2.141124
		C	1.527269	3.385330	0.964799
		H	1.177662	3.818664	1.911678
		H	1.546422	4.174732	0.198991
		C	3.611272	0.287755	0.496403
		C	3.913543	-0.465823	1.655752
		C	3.125236	-0.313222	2.933621
		H	3.454258	-1.048247	3.679571
		H	2.044385	-0.454441	2.771121
		H	3.260904	0.685250	3.379703
		C	4.962234	-1.392969	1.576821
		H	5.204090	-1.985797	2.463446
		C	5.724374	-1.562285	0.408614
		C	6.887226	-2.522965	0.377708
		H	7.810903	-2.018305	0.705951
		H	7.070826	-2.907421	-0.635461
		H	6.728001	-3.376027	1.052438
		C	5.401792	-0.783107	-0.712623
		H	5.993265	-0.889736	-1.626289
		C	4.362844	0.160731	-0.694018
		C	4.075456	1.005893	-1.909270
		H	4.795776	0.789550	-2.708827
		H	4.148802	2.080878	-1.680176
		H	3.061749	0.828097	-2.302046
		C	-0.813470	2.497680	0.335252
		C	-1.272677	3.034382	-0.895668
		C	-0.338487	3.505702	-1.982592
		H	-0.758713	3.299505	-2.976167
Zero-point correction= 0.598303 (Hartree/Particle) Thermal correction to Energy= 0.641009 Thermal correction to Enthalpy= 0.641953 Thermal correction to Gibbs Free Energy= 0.515810 Sum of electronic and Zero-point Energies= -2419.746151 Sum of electronic and thermal Energies= -2419.703445 Sum of electronic and thermal Enthalpies= -2419.702501 Sum of electronic and thermal Free Energies= -2419.828644					

Table S1. Cont.

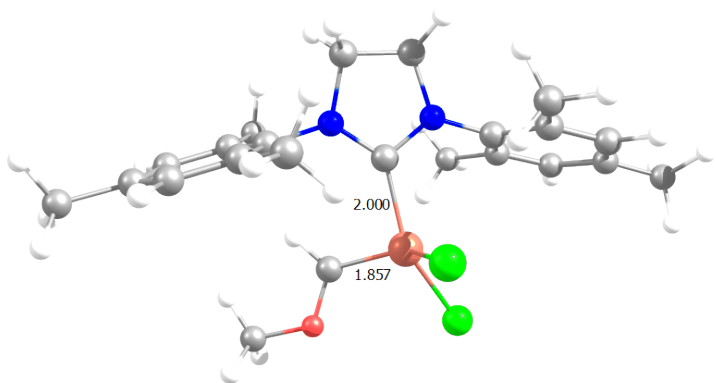
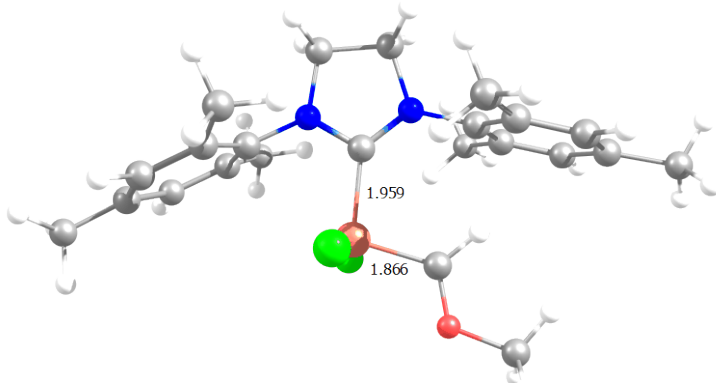
Rh-VITZVPd					
		Rh	-0.347373	1.146747	0.312040
		Cl	-1.642226	3.063011	-0.102473
		Cl	-0.601545	0.716360	2.660746
		N	1.108528	-1.534122	-0.359243
		N	-1.090273	-1.571521	-0.305927
		C	-0.002843	-0.771245	-0.139566
		C	0.776971	-2.966847	-0.580514
		H	1.079898	-3.556259	0.300758
		H	1.311861	-3.358153	-1.457437
		C	-0.745531	-2.934075	-0.770485
		H	-1.044919	-3.056036	-1.825726
		H	-1.269602	-3.693992	-0.174235
		C	2.490560	-1.172683	-0.198894
		C	3.266107	-0.950380	-1.358530
		C	2.660479	-1.031014	-2.740688
		H	3.327122	-0.573820	-3.485035
		H	1.683503	-0.527911	-2.792692
		H	2.498060	-2.077161	-3.050927
		C	4.625372	-0.638689	-1.204488
		H	5.227861	-0.451774	-2.098718
		C	5.228155	-0.565661	0.058949
		C	6.700460	-0.259267	0.203439
		H	7.283242	-1.185045	0.342614
		H	6.894923	0.380343	1.077105
		H	7.096891	0.247131	-0.688359
		C	4.434217	-0.820291	1.186044
		H	4.888531	-0.780012	2.180528
		C	3.071717	-1.140356	1.088444
		C	2.271197	-1.446603	2.326460
		H	2.916182	-1.431106	3.215594
		H	1.806514	-2.444265	2.267305
		H	1.452396	-0.724200	2.479879
		C	-2.462154	-1.128646	-0.325689
		C	-3.289704	-1.438863	0.775880
		C	-2.747001	-2.126874	2.001766
		H	-3.551014	-2.311462	2.727456
Zero-point correction= 0.466561 (Hartree/Particle) Thermal correction to Energy= 0.502152 Thermal correction to Enthalpy= 0.503096 Thermal correction to Gibbs Free Energy= 0.393283 Sum of electronic and Zero-point Energies= -2110.339741 Sum of electronic and thermal Energies= -2110.304150 Sum of electronic and thermal Enthalpies= -2110.303206 Sum of electronic and thermal Free Energies= -2110.413019					
Rh-VITZVP+					
		Rh	-0.338997	1.126015	-0.015166
		Cl	-0.622318	1.377252	-2.295597
		Cl	-0.550147	1.459513	2.259660
		N	0.982274	-1.610465	0.048974
		N	-1.234025	-1.537609	0.049706
		C	-0.101520	-0.818578	0.026229
		C	0.584500	-3.051984	0.085346
		H	1.001861	-3.524072	0.985456
		H	0.987980	-3.565035	-0.798537
		C	-0.960857	-2.996907	0.095674
		H	-1.412657	-3.485487	-0.779035
		H	-1.398417	-3.426809	1.007817
		C	2.372562	-1.236010	0.025656
		C	3.025172	-1.112625	-1.221226
		C	2.298166	-1.332728	-2.525964
		H	2.965484	-1.141054	-3.376055
		H	1.422473	-0.672485	-2.627563
		H	1.939136	-2.370109	-2.620435
		C	4.382002	-0.754803	-1.214355
		H	4.900519	-0.653637	-2.171727
		C	5.093099	-0.543452	-0.021840
		C	6.565353	-0.214919	-0.044889
		H	7.165037	-1.138846	0.001405
		H	6.857113	0.403602	0.815665
		H	6.850576	0.311249	-0.966649
		C	4.406913	-0.689189	1.194716
		H	4.945768	-0.536995	2.134037
		C	3.050665	-1.044722	1.250246
		C	2.351898	-1.193669	2.579738
		H	3.044459	-0.981785	3.404499
		H	1.971476	-2.217095	2.726730
		H	1.494078	-0.509183	2.673140
		C	-2.563949	-0.966285	0.026843
		C	-3.228519	-0.713761	1.253666
		C	-2.662323	-1.119608	2.591240
		H	-2.909127	-0.377848	3.362504
Zero-point correction= 0.468673 (Hartree/Particle) Thermal correction to Energy= 0.504069 Thermal correction to Enthalpy= 0.505013 Thermal correction to Gibbs Free Energy= 0.397041 Sum of electronic and Zero-point Energies= -2110.134490 Sum of electronic and thermal Energies= -2110.099095 Sum of electronic and thermal Enthalpies= -2110.098150 Sum of electronic and thermal Free Energies= -2110.206122					



Table S1. Cont.

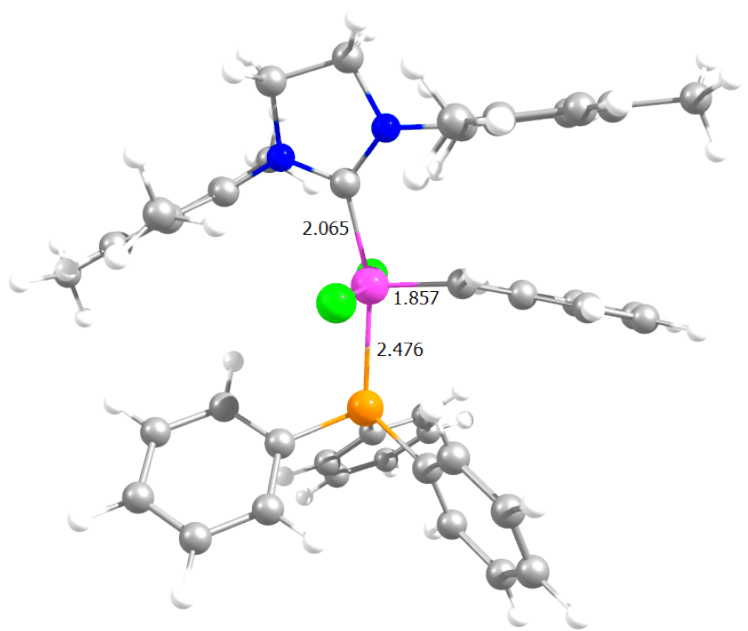
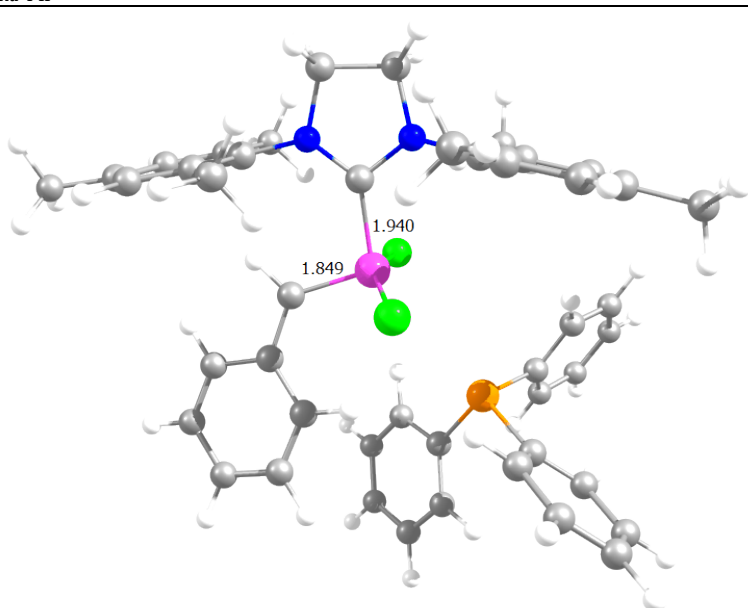
Ru-I		
		
Zero-point correction=	0.781132 (Hartree/Particle)	
Thermal correction to Energy=	0.835682	
Thermal correction to Enthalpy=	0.836626	
Thermal correction to Gibbs Free Energy=	0.687548	
Sum of electronic and Zero-point Energies=	-3247.502187	
Sum of electronic and thermal Energies=	-3247.447637	
Sum of electronic and thermal Enthalpies=	-3247.446692	
Sum of electronic and thermal Free Energies=	-3247.595770	
Ru	0.030857	-0.298599 -0.073068
Cl	-0.257592	-0.346407 2.322858
Cl	-0.182789	-0.446325 -2.507387
P	-1.181151	1.858174 -0.180370
N	-0.371079	-3.319889 -0.097146
N	1.756614	-2.857062 -0.382767
C	0.535895	-2.299634 -0.138810
C	0.216616	-4.631016 -0.463974
H	-0.125733	-4.925800 -1.469651
H	-0.097242	-5.404350 0.251753
C	1.718355	-4.341017 -0.421907
H	2.207040	-4.751358 0.478395
H	2.254156	-4.715963 -1.305179
C	-1.781461	-3.268681 0.197357
C	-2.193154	-3.450501 1.540620
C	-1.198490	-3.650082 2.654160
H	-1.713338	-3.939498 3.580886
H	-0.634593	-2.722742 2.842334
H	-0.469240	-4.438809 2.409188
C	-3.565843	-3.475866 1.817351
H	-3.887508	-3.599456 2.855727
C	-4.531261	-3.375757 0.805271
C	-6.004695	-3.380767 1.139031
H	-6.616414	-3.618243 0.256648
H	-6.328850	-2.395636 1.514282
H	-6.236902	-4.116393 1.924053
C	-4.088746	-3.277056 -0.518601
H	-4.822745	-3.245651 -1.329451
C	-2.724922	-3.240244 -0.853864
C	-2.317912	-3.241492 -2.305812
H	-3.140087	-2.874637 -2.935992
H	-2.085612	-4.267750 -2.641003
H	-1.440233	-2.607508 -2.495027
C	3.053693	-2.240742 -0.349865
C	3.726777	-2.001378 -1.566929
C	3.060896	-2.254666 -2.896067
H	3.699892	-1.906951 -3.719943
H	2.086936	-1.742141 -2.962617
H	2.871340	-3.329331 -3.058338
C	5.038753	-1.507358 -1.509564
H	5.565695	-1.310482 -2.448264
C	5.691685	-1.268873 -0.293199
C	7.095105	-0.712277 -0.256955
H	7.715937	-1.233476 0.487800
H	7.085045	0.355260 0.018616
H	7.588664	-0.799967 -1.235505
C	4.999646	-1.540750 0.895797
H	5.493521	-1.366198 1.856282
C	3.688488	-2.032377 0.895999
C	2.977079	-2.318402 2.193441
H	2.682699	-3.378049 2.271908
H	2.054663	-1.722326 2.288137
H	3.627014	-2.089648 3.049161
C	1.711351	0.454341 -0.309815
C	3.649881	1.955361 -0.207661
C	2.612813	1.286095 0.490556
C	4.558421	2.777324 0.459241
C	2.541259	1.455238 1.892996
C	4.473474	2.927244 1.848572
H	5.336682	3.298462 -0.103258
C	3.468430	2.256075 2.559468
H	1.752222	0.935627 2.441098
H	5.188612	3.562635 2.376594
H	3.406057	2.363425 3.645195
C	-2.807451	1.607077 -1.044246
C	-3.249898	2.449524 -2.075160
C	-3.614338	0.528062 -0.643667
C	-4.486331	2.222864 -2.689864
H	-2.626324	3.282254 -2.404079
C	-4.853600	0.311617 -1.252922
H	-3.280168	-0.145401 0.150104
C	-5.292767	1.157539 -2.277720
H	-4.817690	2.883420 -3.494496
H	-5.470660	-0.528897 -0.929555
H	-6.258547	0.982675 -2.757467
C	-0.402082	3.266532 -1.124988
C	-0.581448	4.603128 -0.728677
C	0.354296	2.986158 -2.275714
C	-0.004886	5.642087 -1.468437
H	-1.168056	4.835939 0.161154
C	0.920397	4.029475 -3.015273
H	0.476019	1.948329 -2.598583
C	0.747036	5.358655 -2.612983
H	-0.146019	6.676166 -1.145232



Table S1. Cont.

Ru-I					
		H	1.501519	3.798789	-3.911372
		H	1.196131	6.170875	-3.189474
		C	-1.684052	2.685856	1.410337
		C	-3.022760	2.949811	1.737008
		C	-0.673074	3.058419	2.313253
		C	-3.344505	3.581604	2.944846
		H	-3.820285	2.666778	1.048578
		C	-0.996335	3.697772	3.512124
		H	0.371961	2.852366	2.075632
		C	-2.333759	3.958822	3.833384
		H	-4.391193	3.781126	3.186386
		H	-0.200071	3.983303	4.203249
		H	-2.585970	4.452438	4.774752
		H	3.725204	1.823050	-1.289692
		H	2.104324	0.318087	-1.335647
Ru-I-II					
		Ru	-0.927617	-0.167812	-0.091135
		Cl	-0.380406	-0.486282	-2.347989
		Cl	-0.421952	-0.039715	2.198125
		P	2.853973	0.722765	0.156837
		N	-2.004933	-2.842619	0.200587
		N	-3.664612	-1.402892	0.412010
		C	-2.317963	-1.499598	0.147348
		C	-3.123485	-3.671982	0.690847
		H	-2.953997	-3.958136	1.743286
		H	-3.214735	-4.588217	0.090257
		C	-4.316159	-2.727980	0.533446
		H	-4.908554	-2.943753	-0.373411
		H	-4.994452	-2.741084	1.398304
		C	-0.745908	-3.473037	-0.101280
		C	-0.521975	-3.916216	-1.427116
		C	-1.554894	-3.721661	-2.507841
		H	-1.240713	-4.223580	-3.433453
		H	-1.696945	-2.653953	-2.728618
		H	-2.531930	-4.138126	-2.212524
		C	0.675132	-4.582776	-1.713147
		H	0.858937	-4.912325	-2.739926
		C	1.630095	-4.853823	-0.722846
		C	2.933463	-5.533578	-1.067963
		H	3.337386	-6.091080	-0.210221
		H	3.693559	-4.792658	-1.366748
		H	2.812476	-6.233477	-1.907971
		C	1.339940	-4.474000	0.592912
		H	2.046273	-4.723540	1.390630
		C	0.155055	-3.803001	0.936016
		C	-0.148646	-3.527877	2.387370
		H	0.778330	-3.491379	2.976343
		H	-0.772973	-4.334332	2.810379
		H	-0.669390	-2.572163	2.528934
		C	-4.540207	-0.267117	0.348516
		C	-4.933163	0.354400	1.552596
		C	-4.345833	-0.067509	2.876586
		H	-4.743266	0.553247	3.691423
		H	-3.247756	0.020192	2.873229
		H	-4.580877	-1.118424	3.112101
		C	-5.858747	1.406601	1.482429
		H	-6.161063	1.902304	2.409794
		C	-6.400845	1.839069	0.264132
		C	-7.425088	2.948758	0.218613
		H	-8.449195	2.539103	0.214697
		H	-7.315970	3.560239	-0.689220
		H	-7.340536	3.611568	1.091902
		C	-5.987163	1.196121	-0.912280
		H	-6.389010	1.527824	-1.874374
		C	-5.065754	0.140463	-0.897848
		C	-4.610589	-0.497181	-2.187171
		H	-4.800467	-1.582243	-2.200835
		H	-3.528280	-0.358638	-2.338641
		H	-5.136728	-0.054887	-3.044137
		C	-1.948939	1.364938	-0.251946
		C	-2.321771	3.793187	-0.406478
		C	-1.481481	2.678943	-0.667773
		C	-1.942357	5.081033	-0.778481
		C	-0.253549	2.911410	-1.334007
		C	-0.720413	5.288784	-1.432889
		H	-2.600359	5.926662	-0.564881
		C	0.116635	4.200488	-1.712268
		H	0.389813	2.063841	-1.575218
		H	-0.423588	6.297085	-1.730474
		H	1.066721	4.360539	-2.225787
		C	3.842279	-0.050287	1.538377
		C	4.661358	0.670755	2.423044
		C	3.736263	-1.444393	1.695102
		C	5.370323	0.009622	3.433486



Zero-point correction= 0.779424 (Hartree/Particle)  
 Thermal correction to Energy= 0.834154  
 Thermal correction to Enthalpy= 0.835098  
 Thermal correction to Gibbs Free Energy= 0.681000  
 Sum of electronic and Zero-point Energies= -3247.486146  
 Sum of electronic and thermal Energies= -3247.431415  
 Sum of electronic and thermal Enthalpies= -3247.430471  
 Sum of electronic and thermal Free Energies= -3247.584570

Ru	-0.927617	-0.167812	-0.091135
Cl	-0.380406	-0.486282	-2.347989
Cl	-0.421952	-0.039715	2.198125
P	2.853973	0.722765	0.156837
N	-2.004933	-2.842619	0.200587
N	-3.664612	-1.402892	0.412010
C	-2.317963	-1.499598	0.147348
C	-3.123485	-3.671982	0.690847
H	-2.953997	-3.958136	1.743286
H	-3.214735	-4.588217	0.090257
C	-4.316159	-2.727980	0.533446
H	-4.908554	-2.943753	-0.373411
H	-4.994452	-2.741084	1.398304
C	-0.745908	-3.473037	-0.101280
C	-0.521975	-3.916216	-1.427116
C	-1.554894	-3.721661	-2.507841
H	-1.240713	-4.223580	-3.433453
H	-1.696945	-2.653953	-2.728618
H	-2.531930	-4.138126	-2.212524
C	0.675132	-4.582776	-1.713147
H	0.858937	-4.912325	-2.739926
C	1.630095	-4.853823	-0.722846
C	2.933463	-5.533578	-1.067963
H	3.337386	-6.091080	-0.210221
H	3.693559	-4.792658	-1.366748
H	2.812476	-6.233477	-1.907971
C	1.339940	-4.474000	0.592912
H	2.046273	-4.723540	1.390630
C	0.155055	-3.803001	0.936016
C	-0.148646	-3.527877	2.387370
H	0.778330	-3.491379	2.976343
H	-0.772973	-4.334332	2.810379
H	-0.669390	-2.572163	2.528934
C	-4.540207	-0.267117	0.348516
C	-4.933163	0.354400	1.552596
C	-4.345833	-0.067509	2.876586
H	-4.743266	0.553247	3.691423
H	-3.247756	0.020192	2.873229
H	-4.580877	-1.118424	3.112101
C	-5.858747	1.406601	1.482429
H	-6.161063	1.902304	2.409794
C	-6.400845	1.839069	0.264132
C	-7.425088	2.948758	0.218613
H	-8.449195	2.539103	0.214697
H	-7.315970	3.560239	-0.689220
H	-7.340536	3.611568	1.091902
C	-5.987163	1.196121	-0.912280
H	-6.389010	1.527824	-1.874374
C	-5.065754	0.140463	-0.897848
C	-4.610589	-0.497181	-2.187171
H	-4.800467	-1.582243	-2.200835
H	-3.528280	-0.358638	-2.338641
H	-5.136728	-0.054887	-3.044137
C	-1.948939	1.364938	-0.251946
C	-2.321771	3.793187	-0.406478
C	-1.481481	2.678943	-0.667773
C	-1.942357	5.081033	-0.778481
C	-0.253549	2.911410	-1.334007
C	-0.720413	5.288784	-1.432889
H	-2.600359	5.926662	-0.564881
C	0.116635	4.200488	-1.712268
H	0.389813	2.063841	-1.575218
H	-0.423588	6.297085	-1.730474
H	1.066721	4.360539	-2.225787
C	3.842279	-0.050287	1.538377
C	4.661358	0.670755	2.423044
C	3.736263	-1.444393	1.695102
C	5.370323	0.009622	3.433486

Table S1. *Cont.*

Ru-I-II				
	H	4.743644	1.755047	2.324607
	C	4.454556	-2.104139	2.696153
	H	3.082044	-2.014092	1.029604
	C	5.273030	-1.378802	3.570557
	H	6.002502	0.584555	4.114753
	H	4.367333	-3.188226	2.802453
	H	5.827112	-1.893412	4.358985
	C	3.033636	2.537530	0.539891
	C	3.884229	3.414597	-0.152828
	C	2.205781	3.052233	1.557648
	C	3.920820	4.775509	0.177830
	H	4.522746	3.033731	-0.952368
	C	2.257131	4.406875	1.895874
	H	1.514980	2.385170	2.081567
	C	3.114002	5.273675	1.205815
	H	4.588521	5.446209	-0.368916
	H	1.613910	4.789913	2.691563
	H	3.147082	6.334519	1.464853
	C	4.008859	0.485490	-1.289491
	C	5.409011	0.416903	-1.176139
	C	3.419690	0.346295	-2.559091
	C	6.203638	0.232721	-2.312601
	H	5.878852	0.499418	-0.193407
	C	4.217257	0.168925	-3.695875
	H	2.329708	0.350302	-2.651381
	C	5.609778	0.113016	-3.575351
	H	7.290550	0.180101	-2.211262
	H	3.745770	0.060020	-4.675468
	H	6.232154	-0.033093	-4.461413
	H	-3.278101	3.624312	0.095557
	H	-3.001250	1.357413	0.061069

Table S1. Cont.

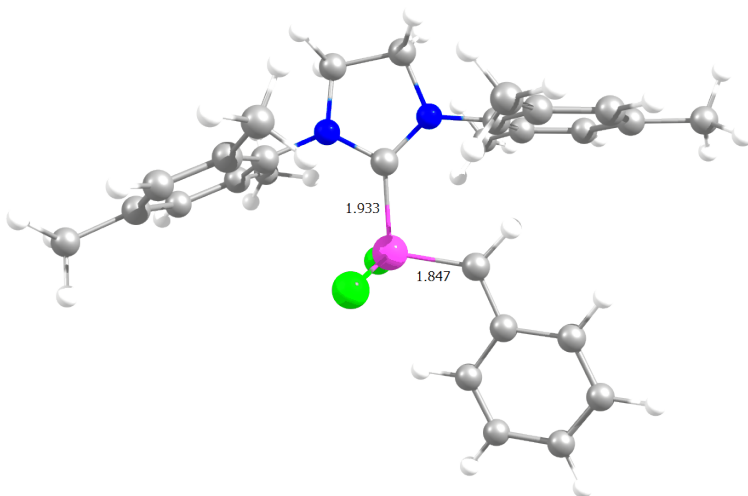
Ru-II					
		Ru	-0.228253	0.906791	0.085788
		Cl	-0.376060	1.238734	2.387216
Zero-point correction= 0.514198 (Hartree/Particle) Thermal correction to Energy= 0.551105 Thermal correction to Enthalpy= 0.552049 Thermal correction to Gibbs Free Energy= 0.440598 Sum of electronic and Zero-point Energies= -2211.214928 Sum of electronic and thermal Energies= -2211.178021 Sum of electronic and thermal Enthalpies= -2211.177077 Sum of electronic and thermal Free Energies= -2211.288528		Cl	-0.998424	1.565050	-2.004403
		N	-1.804914	-1.517052	0.204079
		N	0.334620	-2.068650	0.217082
		C	-0.528071	-1.002684	0.126511
		C	-1.824349	-2.957524	0.522647
		H	-2.544065	-3.483359	-0.121523
		H	-2.120261	-3.113781	1.574449
		C	-0.371512	-3.370035	0.260440
		H	0.046231	-4.002030	1.057194
		H	-0.251002	-3.902190	-0.699508
		C	-3.044297	-0.801887	0.044972
		C	-3.761946	-0.354941	1.176589
		C	-3.307058	-0.638474	2.586652
		H	-3.715810	0.107377	3.282479
		H	-2.214668	-0.619331	2.685129
		H	-3.671989	-1.627076	2.916677
		C	-4.976476	0.316977	0.965334
		H	-5.524604	0.689156	1.836121
		C	-5.509897	0.508694	-0.313890
		C	-6.794815	1.275731	-0.515781
		H	-7.392253	0.852165	-1.336934
		H	-6.585089	2.327276	-0.773769
		H	-7.411844	1.276834	0.394442
		C	-4.813835	-0.026617	-1.407827
		H	-5.234156	0.074461	-2.412761
		C	-3.593101	-0.693203	-1.255449
		C	-2.902973	-1.292531	-2.454802
		H	-3.557814	-1.247454	-3.336037
		H	-2.633840	-2.347496	-2.285511
		H	-1.978990	-0.742680	-2.688944
		C	1.760168	-2.100420	0.060634
		C	2.314810	-2.206459	-1.233564
		C	1.448481	-2.141682	-2.468113
		H	2.056977	-2.265424	-3.374390
		H	0.924064	-1.175126	-2.536915
		H	0.675582	-2.926261	-2.474213
		C	3.708018	-2.316614	-1.349374
		H	4.147235	-2.390828	-2.348822
		C	4.548232	-2.330259	-0.226419
		C	6.043012	-2.488395	-0.377585
		H	6.334418	-3.550539	-0.318043
		H	6.586188	-1.955965	0.416815
		H	6.392677	-2.107509	-1.348137
		C	3.961549	-2.218736	1.042317
		H	4.600844	-2.214022	1.930163
		C	2.574106	-2.107949	1.212811
		C	1.975890	-1.961144	2.589310
		H	1.264680	-2.772293	2.814721
		H	1.420530	-1.014533	2.681661
		H	2.761125	-1.980463	3.357479
		C	1.596970	1.023110	-0.171581
		C	3.676251	2.297365	-0.572299
		C	2.331833	2.278220	-0.123036
		C	4.417970	3.477974	-0.569266
		C	1.769184	3.491643	0.346336
		C	3.839686	4.667831	-0.109074
		H	5.451598	3.472599	-0.922907
		C	2.514786	4.667860	0.350407
		H	0.746377	3.500635	0.732099
		H	4.420532	5.592825	-0.102737
		H	2.065261	5.592555	0.718728
		H	4.125302	1.366796	-0.928985
		H	2.202499	0.147370	-0.440042

Table S1. Cont.

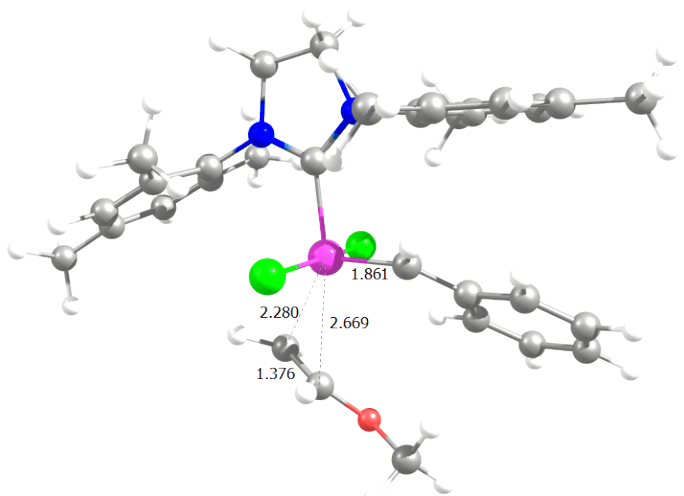
Ru-II-III					
		Ru	-0.234413	0.413977	0.049851
		Cl	-0.490477	0.637197	2.369763
Zero-point correction= 0.597129 (Hartree/Particle) Thermal correction to Energy= 0.640231 Thermal correction to Enthalpy= 0.641175 Thermal correction to Gibbs Free Energy= 0.515475 Sum of electronic and Zero-point Energies= -2404.311286 Sum of electronic and thermal Energies= -2404.268184 Sum of electronic and thermal Enthalpies= -2404.267240 Sum of electronic and thermal Free Energies= -2404.392940		Cl	-0.788716	0.785889	-2.211616
		N	-1.452571	-2.213597	0.013162
		N	0.738527	-2.473379	0.029693
		C	-0.255769	-1.526465	0.008996
		C	-1.279729	-3.665602	0.213350
		H	-1.924680	-4.230423	-0.475086
		H	-1.546812	-3.944002	1.247747
		C	0.213352	-3.854632	-0.070706
		H	0.714021	-4.506064	0.659905
		H	0.398433	-4.260010	-1.080528
		C	-2.776539	-1.646791	0.039053
		C	-3.420233	-1.391245	1.271047
		C	-2.814134	-1.768402	2.600159
		H	-3.108775	-1.053277	3.380299
		H	-1.719258	-1.785396	2.573297
		H	-3.178014	-2.764093	2.910106
		C	-4.712004	-0.842065	1.241506
		H	-5.203384	-0.614849	2.192399
		C	-5.390614	-0.597017	0.042741
		C	-6.759031	0.040945	0.037802
		H	-7.389957	-0.364868	-0.767055
		H	-6.681795	1.128936	-0.124732
		H	-7.279075	-0.112378	0.994471
		C	-4.762870	-0.961134	-1.158031
		H	-5.296961	-0.830299	-2.103812
		C	-3.472277	-1.502432	-1.186967
		C	-2.869200	-1.950339	-2.493774
		H	-3.608318	-1.871165	-3.303172
		H	-2.533115	-2.998788	-2.444028
		H	-1.998239	-1.332284	-2.758949
		C	2.160066	-2.302037	-0.060458
		C	2.778380	-2.278913	-1.329357
		C	1.964007	-2.289802	-2.600438
		H	2.611217	-2.134302	-3.474403
		H	1.197900	-1.498158	-2.593376
		H	1.439529	-3.248461	-2.745612
		C	4.176941	-2.183669	-1.379933
		H	4.665725	-2.151560	-2.358495
		C	4.959987	-2.116426	-0.218289
		C	6.466977	-2.048987	-0.301822
		H	6.797735	-1.590095	-1.244903
		H	6.909468	-3.058284	-0.255361
		H	6.891099	-1.468328	0.530422
		C	4.309083	-2.137611	1.023551
		H	4.901669	-2.071924	1.940851
		C	2.914471	-2.235546	1.129700
		C	2.240398	-2.231749	2.478762
		H	1.616102	-3.128281	2.623705
		H	1.577093	-1.358914	2.591511
		H	2.986446	-2.206708	3.284980
		C	1.578064	0.749944	-0.083438
		C	3.534054	2.231752	-0.314851
		C	2.213218	2.036650	0.166185
		C	4.197789	3.441639	-0.120870
		C	1.594360	3.099947	0.869440
		C	3.565850	4.483300	0.572200
		H	5.212874	3.574305	-0.502562
		C	2.267243	4.304524	1.068713
		H	0.593553	2.959428	1.281174
		H	4.088304	5.429298	0.732843
		H	1.776162	5.109456	1.619646
		C	-1.847670	3.772652	-0.526540
		C	-2.360454	2.942309	0.394760
		H	-2.853637	2.028444	0.067023
		H	-2.345476	3.172834	1.459756
		H	-1.845484	3.520025	-1.592962
		O	-1.290061	4.977319	-0.199077
		C	-0.640727	5.649174	-1.290170
		H	-0.312542	6.621206	-0.902611
		H	0.234838	5.080070	-1.642878
		H	-1.340046	5.809676	-2.128781
		H	4.026097	1.413215	-0.846641
		H	2.268617	-0.013014	-0.467435

Table S1. Cont.

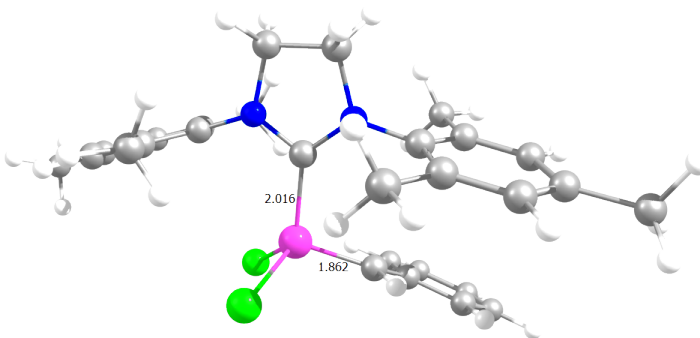
Ru-III					
		Ru	-0.359707	0.603387	-0.859840
		Cl	-1.531775	2.608520	-0.602707
Zero-point correction= 0.512787 (Hartree/Particle) Thermal correction to Energy= 0.550292 Thermal correction to Enthalpy= 0.551236 Thermal correction to Gibbs Free Energy= 0.437705 Sum of electronic and Zero-point Energies= -2211.185941 Sum of electronic and thermal Energies= -2211.148436 Sum of electronic and thermal Enthalpies= -2211.147492 Sum of electronic and thermal Free Energies= -2211.261023		Cl	-0.816863	-0.346755	-2.981163
		N	-1.674085	-1.384131	0.892557
		N	0.493675	-1.783456	0.899451
		C	-0.473577	-0.952443	0.416524
		C	-1.553440	-2.538076	1.812158
		H	-2.224217	-3.352231	1.500296
		H	-1.834116	-2.236886	2.835256
		C	-0.065561	-2.908902	1.690809
		H	0.441176	-2.979406	2.664719
		H	0.089309	-3.859498	1.154661
		C	-2.943126	-0.733776	0.693810
		C	-3.326657	0.317139	1.554657
		C	-2.400601	0.840372	2.624103
		H	-2.926269	1.553122	3.274096
		H	-1.545758	1.365495	2.169169
		H	-1.996392	0.036597	3.259069
		C	-4.588026	0.895164	1.369730
		H	-4.887008	1.720034	2.023000
		C	-5.468030	0.454190	0.371549
		C	-6.801834	1.130379	0.163247
		H	-7.538411	0.443021	-0.277490
		H	-6.698740	1.987538	-0.522871
		H	-7.211286	1.515423	1.108748
		C	-5.064569	-0.609079	-0.446484
		H	-5.741124	-0.974306	-1.224686
		C	-3.812391	-1.223350	-0.305091
		C	-3.412874	-2.354981	-1.218361
		H	-4.265845	-2.670380	-1.834885
		H	-3.057562	-3.235360	-0.659843
		H	-2.599739	-2.043302	-1.894602
		C	1.897023	-1.781050	0.595884
		C	2.369871	-2.482086	-0.534254
		C	1.424932	-3.145557	-1.505342
		H	1.985844	-3.659643	-2.297682
		H	0.754022	-2.412225	-1.982668
		H	0.784890	-3.894103	-1.011203
		C	3.754899	-2.521424	-0.752538
		H	4.130680	-3.055084	-1.630763
		C	4.664647	-1.903572	0.117310
		C	6.153265	-1.999635	-0.121053
		H	6.579463	-2.873913	0.399110
		H	6.678984	-1.109094	0.253236
		H	6.383684	-2.111457	-1.190494
		C	4.157099	-1.215910	1.228591
		H	4.848916	-0.713576	1.910930
		C	2.782472	-1.145124	1.490911
		C	2.266446	-0.373981	2.680049
		H	1.623764	-0.991868	3.326947
		H	1.663218	0.488043	2.355415
		H	3.098437	0.002842	3.290254
		C	1.461772	0.986569	-0.895264
		C	3.638521	2.119694	-0.738962
		C	2.263785	2.080399	-0.383319
		C	4.474374	3.131270	-0.269013
		C	1.766164	3.103319	0.463176
		C	3.962031	4.134435	0.563546
		H	5.527710	3.143712	-0.558521
		C	2.605077	4.116224	0.920017
		H	0.706707	3.102490	0.724504
		H	4.614133	4.931610	0.927358
		H	2.200373	4.902786	1.561050
		H	4.035835	1.341276	-1.394866
		H	2.005977	0.291170	-1.560884

Table S1. Cont.

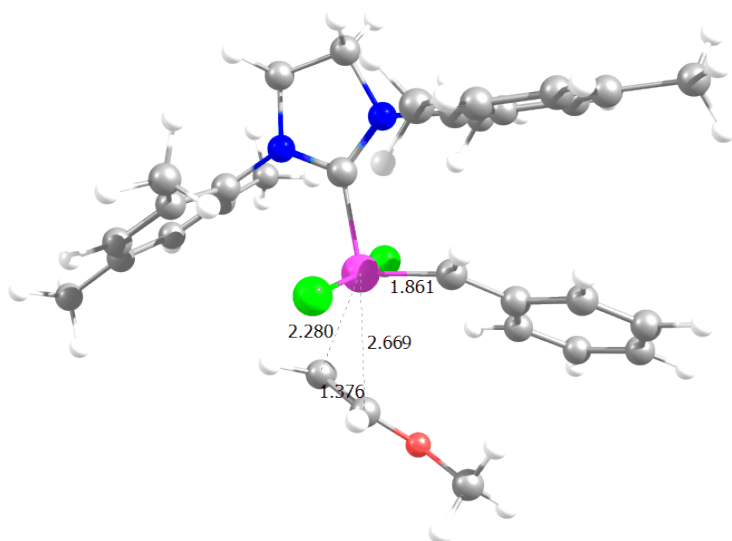
Ru-III					
		Ru	-0.420268	0.738365	-0.196777
		Cl	-0.429014	1.106341	2.181479
Zero-point correction= 0.598571 (Hartree/Particle) Thermal correction to Energy= 0.640444 Thermal correction to Enthalpy= 0.641388 Thermal correction to Gibbs Free Energy= 0.521763 Sum of electronic and Zero-point Energies= -2404.320309 Sum of electronic and thermal Energies= -2404.278435 Sum of electronic and thermal Enthalpies= -2404.277491 Sum of electronic and thermal Free Energies= -2404.397116		Cl	-0.729693	0.491439	-2.608135
		N	-1.942578	-1.741863	0.300783
		N	0.187891	-2.279697	0.191469
		C	-0.686057	-1.239798	0.098878
		C	-1.944190	-3.176608	0.661872
		H	-2.662245	-3.727177	0.036616
		H	-2.235926	-3.302529	1.717441
		C	-0.486946	-3.585051	0.402883
		H	-0.031337	-4.112929	1.253141
		H	-0.377397	-4.217362	-0.493612
		C	-3.184255	-1.008789	0.262224
		C	-3.754167	-0.517763	1.460768
		C	-3.153637	-0.798090	2.815252
		H	-3.539108	-0.089655	3.561424
		H	-2.059729	-0.710390	2.809952
		H	-3.429331	-1.812204	3.154565
		C	-4.964119	0.187685	1.376983
		H	-5.395454	0.591387	2.297832
		C	-5.641262	0.367535	0.164512
		C	-6.918608	1.170646	0.098726
		H	-7.587870	0.799188	-0.691303
		H	-6.705658	2.229530	-0.124701
		H	-7.462544	1.141087	1.054093
		C	-5.103232	-0.226700	-0.985305
		H	-5.647522	-0.154710	-1.931614
		C	-3.895253	-0.937395	-0.961274
		C	-3.409890	-1.636432	-2.204570
		H	-4.175225	-1.589243	-2.991842
		H	-3.191571	-2.698708	-2.009194
		H	-2.487649	-1.171801	-2.588054
		C	1.617132	-2.281521	0.046590
		C	2.181771	-2.554938	-1.217314
		C	1.324907	-2.699893	-2.450422
		H	1.950805	-2.881660	-3.335085
		H	0.720446	-1.795274	-2.633173
		H	0.620152	-3.543086	-2.365222
		C	3.578428	-2.665044	-1.306459
		H	4.026133	-2.874847	-2.282645
		C	4.408303	-2.523957	-0.186594
		C	5.909628	-2.644323	-0.306480
		H	6.403738	-1.684252	-0.085846
		H	6.208247	-2.952055	-1.318576
		H	6.309830	-3.383640	0.405036
		C	3.809848	-2.261477	1.054490
		H	4.440330	-2.147893	1.941377
		C	2.421513	-2.144097	1.200032
		C	1.811856	-1.871166	2.551174
		H	1.119251	-2.674084	2.853322
		H	1.232833	-0.933288	2.551033
		H	2.593737	-1.798121	3.319624
		C	1.417764	0.727181	-0.487327
		C	3.809894	1.267367	-0.511166
		C	2.539427	1.452460	0.099691
		C	4.942257	1.929175	-0.041057
		C	2.456752	2.337251	1.202991
		C	4.838661	2.796459	1.055681
		H	5.907680	1.772871	-0.528164
		C	3.596219	2.991293	1.673170
		H	1.492230	2.484030	1.688318
		H	5.724310	3.317466	1.427459
		H	3.513828	3.664784	2.529532
		C	-1.407677	2.793059	-0.258725
		C	-0.368923	3.275941	-1.021354
		H	-2.265378	2.378445	-0.800304
		H	-1.566240	3.166219	0.753820
		H	-0.269021	3.014605	-2.080881
		O	0.521552	4.155070	-0.519319
		C	1.580187	4.532442	-1.427401
		H	1.160532	5.020879	-2.321527
		H	2.211586	5.240059	-0.879421
		H	2.174141	3.653925	-1.718868
		H	3.887787	0.586711	-1.362741
		H	1.733836	0.121033	-1.354478

Table S1. Cont.

Ru-III-IV				
Zero-point correction=	0.599147 (Hartree/Particle)			
Thermal correction to Energy=	0.640593			
Thermal correction to Enthalpy=	0.641537			
Thermal correction to Gibbs Free Energy=	0.523596			
Sum of electronic and Zero-point Energies=	-2404.309487			
Sum of electronic and thermal Energies=	-2404.268041			
Sum of electronic and thermal Enthalpies=	-2404.267097			
Sum of electronic and thermal Free Energies=	-2404.385038			
Ru	0.243591	-0.882958	-0.089555	
Cl	0.095499	-1.111710	2.327454	
Cl	0.790048	-0.716681	-2.451180	
N	1.719808	1.748432	0.353764	
N	-0.444093	2.092027	0.165909	
C	0.521473	1.138900	0.133900	
C	1.576443	3.192232	0.670198	
H	2.275662	3.786139	0.064294	
H	1.802467	3.367483	1.734775	
C	0.105936	3.461644	0.331256	
H	-0.429187	3.992399	1.131417	
H	-0.018889	4.031078	-0.604916	
C	3.038648	1.165861	0.322587	
C	3.647440	0.731654	1.522822	
C	2.963322	0.853339	2.860718	
H	3.533612	0.318248	3.632774	
H	1.942906	0.443208	2.844050	
H	2.900961	1.909305	3.175041	
C	4.955936	0.227356	1.455062	
H	5.427297	-0.122523	2.378451	
C	5.681162	0.188859	0.257580	
C	7.078274	-0.383592	0.211318	
H	7.694746	0.121053	-0.547129	
H	7.057852	-1.455886	-0.046266	
H	7.584092	-0.290863	1.183461	
C	5.073896	0.700405	-0.897690	
H	5.638463	0.724738	-1.834655	
C	3.766880	1.208066	-0.890626	
C	3.182936	1.803119	-2.145756	
H	3.936433	1.828036	-2.945163	
H	2.833688	2.835529	-1.981896	
H	2.321350	1.211507	-2.495745	
C	-1.858274	1.946962	-0.060251	
C	-2.361417	2.026565	-1.376682	
C	-1.449161	2.153097	-2.570171	
H	-2.036760	2.267603	-3.491755	
H	-0.798227	1.268936	-2.680470	
H	-0.786255	3.029948	-2.488497	
C	-3.752672	1.982780	-1.552359	
H	-4.152349	2.039878	-2.569385	
C	-4.637908	1.884212	-0.471026	
C	-6.129633	1.807147	-0.692727	
H	-6.683242	2.332339	0.099927	
H	-6.468692	0.757826	-0.688701	
H	-6.416275	2.244464	-1.660177	
C	-4.100582	1.837333	0.822530	
H	-4.774990	1.771670	1.681447	
C	-2.719052	1.875343	1.055618	
C	-2.180929	1.843981	2.464110	
H	-1.668916	2.785812	2.724732	
H	-1.452999	1.028692	2.601427	
H	-2.999165	1.705688	3.184428	
C	-1.458446	-1.453483	-0.682811	
C	-3.846250	-1.928515	-0.966044	
C	-2.767140	-1.716673	-0.071985	
C	-5.127705	-2.217899	-0.496066	
C	-3.024160	-1.805472	1.314334	
C	-5.359183	-2.314167	0.881149	
H	-5.943277	-2.381426	-1.204282	
C	-4.303103	-2.109845	1.779650	
H	-2.201155	-1.643248	2.013049	
H	-6.358411	-2.552123	1.253718	
H	-4.480304	-2.187201	2.854919	
C	-0.158777	-3.177204	-0.148211	
C	1.224757	-2.893725	-0.100308	
H	-0.672225	-3.395024	0.787399	
H	-0.523181	-3.665929	-1.054519	
H	1.724420	-2.789155	0.874905	
O	2.008794	-3.308598	-1.131398	
C	3.341952	-2.768324	-1.150764	
H	3.789023	-2.788064	-0.141644	
H	3.921762	-3.408477	-1.826508	
H	3.321425	-1.737886	-1.533734	
H	-3.660485	-1.868595	-2.041558	
H	-1.501796	-1.556568	-1.782095	

Table S1. Cont.

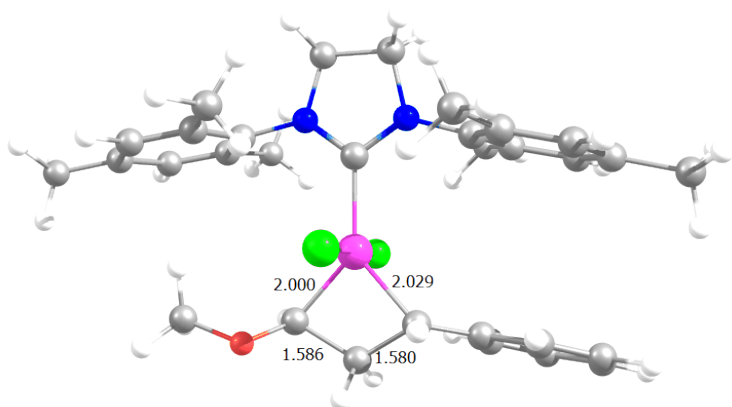
Ru-IV			
		Ru	0.173013 -0.824770 -0.204746
		Cl	-0.024636 -1.283528 2.177176
Zero-point correction= 0.601099 (Hartree/Particle) Thermal correction to Energy= 0.642794 Thermal correction to Enthalpy= 0.643739 Thermal correction to Gibbs Free Energy= 0.524387 Sum of electronic and Zero-point Energies= -2404.319871 Sum of electronic and thermal Energies= -2404.278176 Sum of electronic and thermal Enthalpies= -2404.277231 Sum of electronic and thermal Free Energies= -2404.396583		Cl	0.515163 -0.376059 -2.563308
		N	1.780752 1.667380 0.460107
		N	-0.376341 2.096785 0.306438
		C	0.563628 1.127270 0.195856
		C	1.686624 3.091628 0.873340
		H	2.381103 3.701728 0.277969
		H	1.960450 3.191901 1.935789
		C	0.212249 3.425981 0.609848
		H	-0.289513 3.868811 1.481911
		H	0.074513 4.102179 -0.249037
		C	3.088227 1.063330 0.378091
		C	3.685013 0.531621 1.543666
		C	2.968915 0.510342 2.869429
		H	3.557924 -0.042329 3.614451
		H	1.976813 0.038356 2.793659
		H	2.823261 1.531582 3.260604
		C	4.999511 0.048047 1.450146
		H	5.464578 -0.372827 2.346624
		C	5.737507 0.115887 0.261632
		C	7.143833 -0.430684 0.187012
		H	7.760064 1.039910 -0.523279
		H	7.142824 -1.480172 -0.152341
		H	7.637799 -0.405267 1.169228
		C	5.131220 0.699503 -0.859712
		H	5.699643 0.791572 -1.790028
		C	3.817880 1.191296 -0.826839
		C	3.224340 1.840564 -2.049403
		H	3.979423 1.929800 -2.842554
		H	2.843447 2.851855 -1.832742
		H	2.377120 1.248888 -2.435007
		C	-1.802234 2.004538 0.097672
		C	-2.331122 2.282751 -1.182190
		C	-1.446865 2.585463 -2.364347
		H	-2.055434 2.760915 -3.262329
		H	-0.753786 1.753663 -2.571790
		H	-0.838521 3.490080 -2.197850
		C	-3.726204 2.288663 -1.329779
		H	-4.144862 2.497148 -2.318928
		C	-4.591113 2.058436 -0.252935
		C	-6.088346 2.046640 -0.446996
		H	-6.609415 2.505975 0.406425
		H	-6.460207 1.012461 -0.537131
		H	-6.380820 2.585684 -1.359719
		C	-4.029462 1.829003 1.010005
		H	-4.687354 1.669217 1.869093
		C	-2.643618 1.809923 1.216462
		C	-2.089590 1.604564 2.602628
		H	-1.453114 2.448301 2.917043
		H	-1.472748 0.693243 2.658297
		H	-2.907070 1.516331 3.331458
		C	-1.401857 -1.929529 -0.849576
		C	-3.857854 -1.763911 -1.030657
		C	-2.738889 -2.062760 -0.222283
		C	-5.159678 -1.921610 -0.550629
		C	-2.972098 -2.513816 1.093491
		C	-5.373596 -2.379605 0.753836
		H	-6.008502 -1.698258 -1.201317
		C	-4.273459 -2.671130 1.571430
		H	-2.123529 -2.707471 1.750926
		H	-6.390114 -2.509345 1.132522
		H	-4.431883 -3.022428 2.593788
		C	-0.296895 -3.019150 -0.552036
		C	1.191568 -2.543994 -0.281126
		H	-0.609377 -3.616137 0.311688
		H	-0.203975 -3.602295 -1.478192
		H	1.562899 -2.825264 0.719384
		O	2.035456 -2.926788 -1.296143
		C	3.429289 -2.767827 -0.993682
		H	3.674493 -3.221711 -0.016784
		H	3.976937 -3.285801 -1.790161
		H	3.704170 -1.702170 -0.985140
		H	-3.692963 -1.415756 -2.053544
		H	-1.491899 -1.762968 -1.930725



Table S1. Cont.

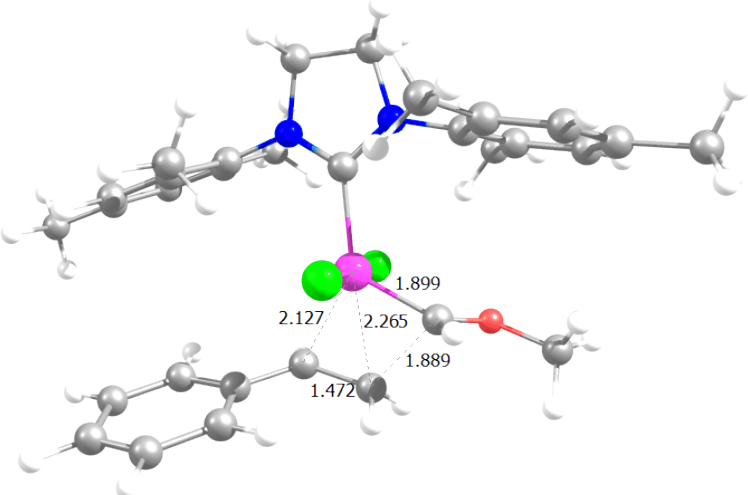
Ru-IV-V					
		Ru	-0.137503	0.695245	-0.433672
		Cl	-0.174001	1.545979	1.841803
Zero-point correction= 0.599463 (Hartree/Particle) Thermal correction to Energy= 0.641034 Thermal correction to Enthalpy= 0.641978 Thermal correction to Gibbs Free Energy= 0.522500 Sum of electronic and Zero-point Energies= -2404.319170 Sum of electronic and thermal Energies= -2404.277599 Sum of electronic and thermal Enthalpies= -2404.276655 Sum of electronic and thermal Free Energies= -2404.396133		Cl	-0.056633	-0.136937	-2.704879
		N	-1.680610	-1.732009	0.586692
		N	0.463825	-2.185265	0.383963
		C	-0.475025	-1.217185	0.234124
		C	-1.605422	-3.181887	0.901314
		H	-2.093828	-3.763321	0.101880
		H	-2.121413	-3.394481	1.848196
		C	-0.093567	-3.430770	0.969918
		H	0.271649	-3.554003	2.003166
		H	0.226295	-4.304147	0.384596
		C	-2.971397	-1.091328	0.571121
		C	-3.493519	-0.598300	1.789049
		C	-2.699175	-0.648084	3.068982
		H	-3.290462	-0.247705	3.904214
		H	-1.775170	-0.054153	2.977907
		H	-2.408414	-1.678674	3.330869
		C	-4.782876	-0.048995	1.781707
		H	-5.187912	0.345443	2.718568
		C	-5.567181	-0.007252	0.619773
		C	-6.971854	0.549763	0.655629
		H	-7.672073	-0.172822	1.107056
		H	-7.340815	0.777561	-0.354750
		H	-7.026056	1.470117	1.256888
		C	-5.028315	-0.534035	-0.560474
		H	-5.630853	-0.529670	-1.473841
		C	-3.741271	-1.093901	-0.612063
		C	-3.221766	-1.673548	-1.901858
		H	-4.008718	-1.668479	-2.668828
		H	-2.885439	-2.715109	-1.775744
		H	-2.358908	-1.104186	-2.284779
		C	1.890254	-2.078665	0.195761
		C	2.458356	-2.603083	-0.989326
		C	1.606078	-3.196573	-2.080957
		H	2.234786	-3.545783	-2.911792
		H	0.894558	-2.450381	-2.469697
		H	1.022410	-4.060104	-1.720886
		C	3.851581	-2.563054	-1.126344
		H	4.296891	-2.957515	-2.044821
		C	4.684572	-2.050286	-0.120751
		C	6.183825	-2.017630	-0.305226
		H	6.693002	-1.684000	0.609893
		H	6.470000	-1.331299	-1.118851
		H	6.577615	-3.011582	-0.570194
		C	4.089469	-1.581141	1.055411
		H	4.722280	-1.197936	1.860898
		C	2.698719	-1.596314	1.248130
		C	2.115716	-1.123502	2.555222
		H	1.450121	-1.879345	3.002348
		H	1.517601	-0.205856	2.430951
		H	2.916892	-0.915004	3.277533
		C	1.346105	2.061974	-1.107756
		C	3.748322	1.871821	-0.564375
		C	2.489905	2.424470	-0.243003
		C	4.894042	2.218017	0.155161
		C	2.419221	3.336799	0.830348
		C	4.807546	3.129366	1.212737
		H	5.857908	1.781290	-0.115714
		C	3.564363	3.684392	1.546052
		H	1.456713	3.757226	1.121192
		H	5.702167	3.408708	1.774058
		H	3.487572	4.393152	2.373813
		C	0.086896	2.820923	-1.183832
		C	-1.532317	1.938030	-0.775039
		H	0.000931	3.648367	-0.473511
		H	-0.213153	3.047323	-2.211198
		H	-1.925277	2.515937	0.082292
		O	-2.366682	1.912474	-1.839109
		C	-3.506041	2.801621	-1.751665
		H	-3.182563	3.853819	-1.804253
		H	-4.136842	2.566616	-2.616442
		H	-4.068385	2.623482	-0.822195
		H	3.817706	1.163653	-1.394139
		H	1.659597	1.639637	-2.069155

Table S1. Cont.

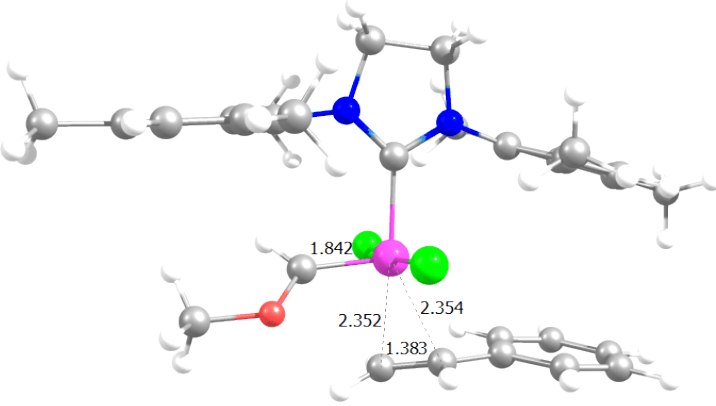
Ru-V					
		Ru	-0.091074	-0.961943	-0.098492
		Cl	0.128480	-0.595736	-2.502292
Zero-point correction= 0.599611 (Hartree/Particle) Thermal correction to Energy= 0.642151 Thermal correction to Enthalpy= 0.643095 Thermal correction to Gibbs Free Energy= 0.520382 Sum of electronic and Zero-point Energies= -2404.328653 Sum of electronic and thermal Energies= -2404.286113 Sum of electronic and thermal Enthalpies= -2404.285169 Sum of electronic and thermal Free Energies= -2404.407883		Cl	-0.176607	-1.161074	2.327664
		N	-1.806081	1.632182	0.278152
		N	0.355383	1.987089	0.394263
		C	-0.587651	1.028850	0.169293
		C	-1.715306	3.095262	0.516080
		H	-2.354610	3.381800	1.363330
		H	-2.060267	3.644954	-0.375909
		C	-0.223627	3.292980	0.795861
		H	0.224637	4.103852	0.204209
		H	-0.014642	3.482878	1.861091
		C	-3.124052	1.091915	0.087329
		C	-3.697409	1.110141	-1.205350
		C	-2.906774	1.542682	-2.414152
		H	-3.533614	1.510062	-3.315976
		H	-2.026902	0.897004	-2.578683
		H	-2.528551	2.572006	-2.307241
		C	-5.027742	0.686645	-1.345221
H	-5.475104	0.689444	-2.343870		
C	-5.799427	0.278736	-0.246957		
C	-7.246152	-0.120672	-0.422814		
H	-7.903350	0.764767	-0.399499		
H	-7.579130	-0.795425	0.379150		
H	-7.412412	-0.622782	-1.387387		
C	-5.201903	0.287125	1.020688		
H	-5.786993	-0.023214	1.891678		
C	-3.874253	0.699273	1.217735		
C	-3.278502	0.719091	2.601379		
H	-4.000208	0.341073	3.338698		
H	-2.999181	1.742018	2.904433		
H	-2.362605	0.107574	2.655679		
C	1.789210	1.910039	0.244826		
C	2.607522	1.720810	1.382077		
C	2.034409	1.536040	2.763837		
H	2.818146	1.212964	3.463277		
H	1.227212	0.788388	2.780573		
H	1.625671	2.485621	3.151271		
C	3.998667	1.768671	1.208515		
H	4.637464	1.607577	2.081760		
C	4.588414	2.040727	-0.031369		
C	6.089179	2.065284	-0.189230		
H	6.398589	2.740896	-1.000259		
H	6.468907	1.059304	-0.434178		
H	6.587448	2.386726	0.737300		
C	3.746094	2.287731	-1.123003		
H	4.184795	2.541230	-2.092696		
C	2.350318	2.247444	-1.010115		
C	1.490924	2.597457	-2.197146		
H	0.780531	3.406640	-1.960575		
H	0.904085	1.725703	-2.528336		
H	2.115584	2.935691	-3.035622		
C	1.347915	-2.793021	0.230601		
C	3.628463	-2.364815	1.092826		
C	2.737065	-2.349846	-0.001457		
C	4.987641	-2.101469	0.914655		
C	3.241650	-2.008017	-1.274446		
C	5.480863	-1.800586	-0.360200		
H	5.665488	-2.140086	1.770565		
C	4.599553	-1.738368	-1.447767		
H	2.560758	-1.944252	-2.125763		
H	6.547447	-1.613702	-0.506271		
H	4.975349	-1.484728	-2.441686		
C	0.436937	-3.164308	-0.742138		
C	-1.809099	-1.599380	-0.286887		
H	0.669909	-3.117351	-1.806237		
H	-0.413375	-3.779918	-0.452136		
H	-2.481935	-1.196337	-1.068400		
O	-2.347867	-2.602316	0.403566		
C	-3.675880	-3.055761	0.016507		
H	-3.578575	-3.869480	-0.716744		
H	-4.151188	-3.428704	0.930772		
H	-4.260085	-2.224605	-0.403506		
H	3.240831	-2.608330	2.085108		
H	1.130843	-3.068342	1.265219		

Table S1. Cont.

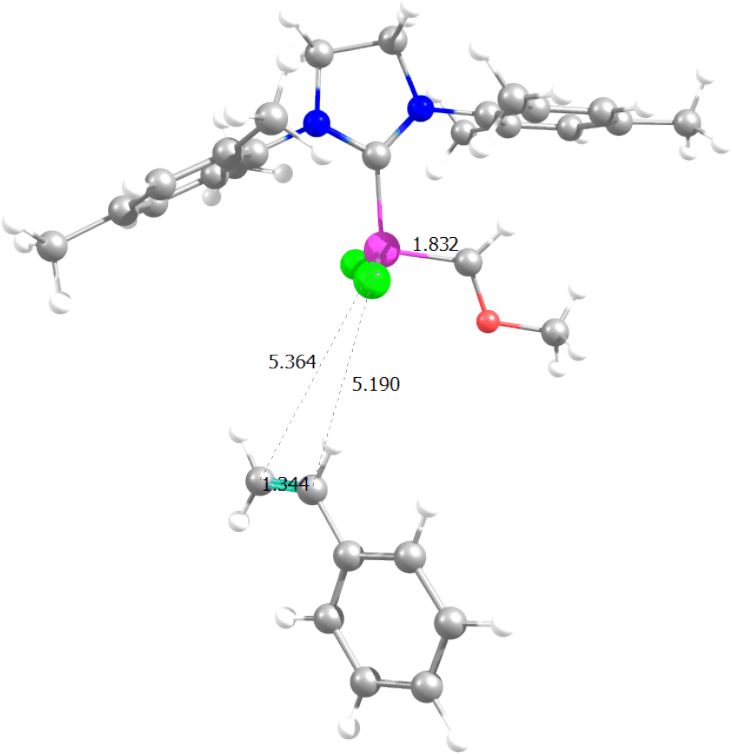
Ru-V-VI				
				
Zero-point correction=	0.596541 (Hartree/Particle)			
Thermal correction to Energy=	0.640249			
Thermal correction to Enthalpy=	0.641193			
Thermal correction to Gibbs Free Energy=	0.508159			
Sum of electronic and Zero-point Energies=	-2404.323518			
Sum of electronic and thermal Energies=	-2404.279810			
Sum of electronic and thermal Enthalpies=	-2404.278865			
Sum of electronic and thermal Free Energies=	-2404.411899			
Ru	0.190222	0.000682	-0.440583	
Cl	-1.096392	0.078345	1.520158	
Cl	0.415129	0.379954	-2.738769	
N	3.141619	0.166049	0.255255	
N	2.041759	2.080200	0.312454	
C	1.894132	0.724830	0.105014	
C	4.154848	1.150864	0.696993	
H	5.083157	1.029051	0.120765	
H	4.390251	1.006700	1.766505	
C	3.454426	2.488307	0.431395	
H	3.580521	3.211092	1.250329	
H	3.800077	2.957709	-0.505945	
C	3.498683	-1.221890	0.276408	
C	3.380757	-1.955342	1.477504	
C	2.765711	-1.343569	2.712824	
H	2.764400	-2.064024	3.542168	
H	1.725771	-1.030379	2.526678	
H	3.314720	-0.449544	3.047888	
C	3.800560	-3.293631	1.479969	
H	3.707615	-3.871508	2.404525	
C	4.331205	-3.908021	0.335623	
C	4.818982	-5.337204	0.380241	
H	5.876770	-5.380766	0.689578	
H	4.747316	-5.819442	-0.605533	
H	4.244428	-5.937816	1.100562	
C	4.425284	-3.150964	-0.841001	
H	4.826178	-3.616298	-1.746515	
C	4.020966	-1.808375	-0.895850	
C	4.105582	-1.028399	-2.183917	
H	4.541961	-1.644082	-2.982500	
H	4.730040	-0.127300	-2.073841	
H	3.108803	-0.688715	-2.509151	
C	0.992934	3.066267	0.302659	
C	0.707479	3.794289	-0.874830	
C	1.505691	3.619588	-2.142696	
H	0.932682	3.971321	-3.011686	
H	1.770951	2.570352	-2.324739	
H	2.434102	4.215943	-2.100085	
C	-0.313735	4.756078	-0.825342	
H	-0.556112	5.306135	-1.739639	
C	-1.014317	5.039921	0.352686	
C	-2.140766	6.045375	0.366417	
H	-2.171940	6.602733	1.314537	
H	-3.115225	5.541684	0.252764	
H	-2.046224	6.769059	-0.456120	
C	-0.644907	4.360026	1.522478	
H	-1.148466	4.598990	2.463754	
C	0.359629	3.385342	1.528199	
C	0.763281	2.722025	2.820427	
H	1.852921	2.768158	2.976646	
H	0.466431	1.662629	2.825529	
H	0.276953	3.216267	3.672895	
C	-4.993501	-0.133780	-0.227649	
C	-5.744553	-2.175588	0.968332	
C	-6.006434	-1.174877	0.009525	
C	-6.670156	-3.189897	1.229477	
C	-7.237586	-1.228544	-0.678706	
C	-7.884334	-3.227417	0.536544	
H	-6.442476	-3.952785	1.977856	
C	-8.162019	-2.239563	-0.419137	
H	-7.473754	-0.468577	-1.426791	
H	-8.610831	-4.017849	0.737804	
H	-9.108462	-2.260285	-0.964960	
C	-5.058588	0.878893	-1.109006	
C	0.542008	-1.797025	-0.441330	
H	-5.914312	1.035924	-1.770417	
H	-4.235482	1.588698	-1.200109	
H	1.451264	-2.314214	-0.091339	
O	-0.407231	-2.621740	-0.909108	
C	-0.195491	-4.051965	-0.787640	
H	-0.680908	-4.411165	0.131071	
H	-0.663692	-4.514658	-1.664242	
H	0.880747	-4.282114	-0.764027	
H	-4.796366	-2.148518	1.512124	
H	-4.092561	-0.217807	0.391506	

Table S1. Cont.

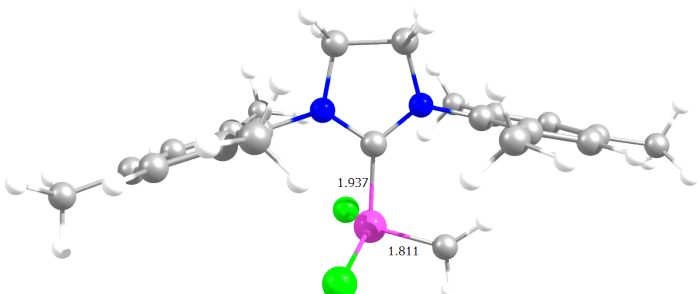
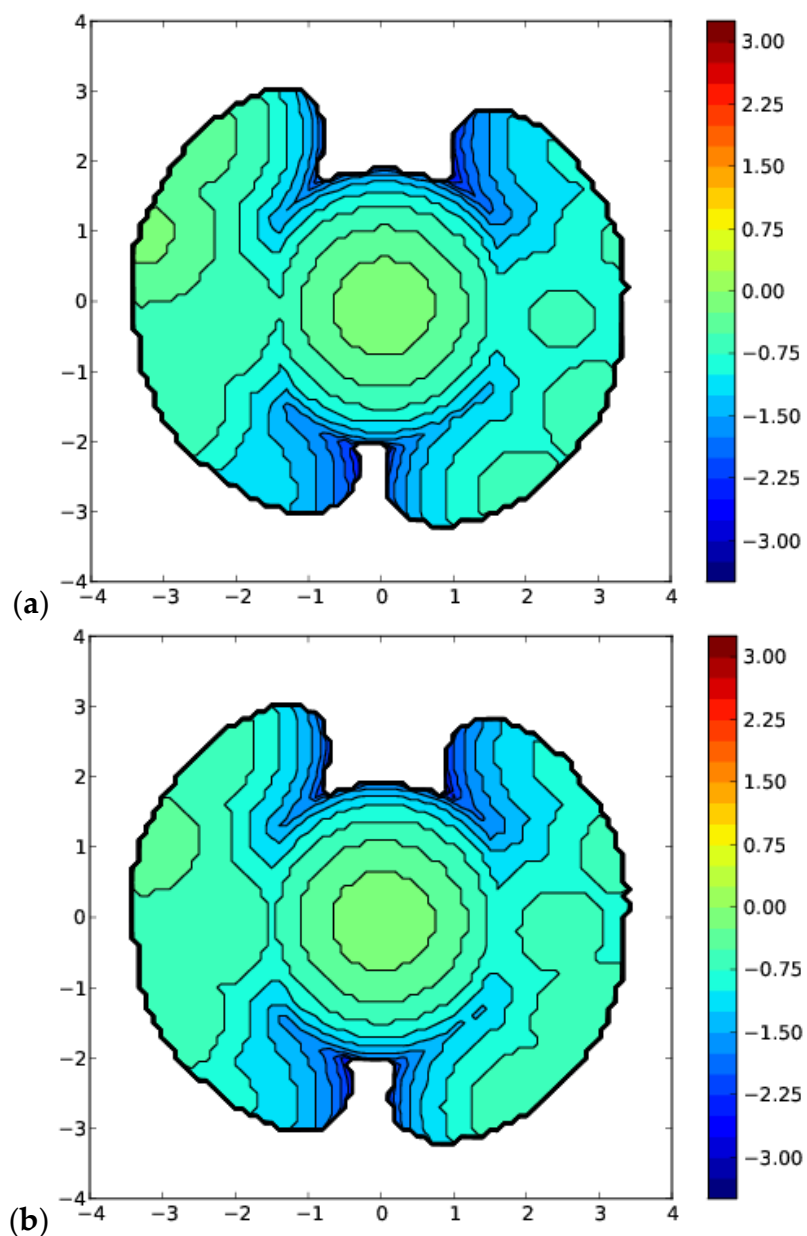
Ru-VI					
		Ru	-0.097077	0.353440	-1.433386
		Cl	-1.028641	-1.597178	-2.278175
Zero-point correction= 0.435280 (Hartree/Particle) Thermal correction to Energy= 0.467033 Thermal correction to Enthalpy= 0.467978 Thermal correction to Gibbs Free Energy= 0.370356 Sum of electronic and Zero-point Energies= -1980.161085 Sum of electronic and thermal Energies= -1980.129331 Sum of electronic and thermal Enthalpies= -1980.128387 Sum of electronic and thermal Free Energies= -1980.226009		Cl	-0.429092	2.640190	-1.197293
		N	1.212061	-0.228614	1.219935
		N	-0.995970	-0.278076	1.271982
		C	0.088414	-0.094496	0.442332
		C	0.895780	-0.634970	2.608078
		H	1.479396	-0.037504	3.322808
		H	1.146297	-1.699217	2.760224
		C	-0.611086	-0.373536	2.694885
		H	-1.162304	-1.186158	3.189212
		H	-0.842229	0.571663	3.216053
		C	2.590797	-0.206202	0.823954
		C	3.216462	-1.403008	0.413179
		C	2.435225	-2.686374	0.266102
		H	3.068030	-3.477313	-0.158912
		H	1.564265	-2.550309	-0.393587
		H	2.056161	-3.051229	1.234693
		C	4.580061	-1.358156	0.088635
		H	5.070357	-2.276911	-0.246933
		C	5.325115	-0.172866	0.171673
		C	6.799876	-0.159250	-0.154775
		H	7.405081	-0.337511	0.749967
		H	7.110970	0.810460	-0.569923
		H	7.058485	-0.942828	-0.881564
		C	4.669535	0.995120	0.586262
		H	5.231248	1.932051	0.646891
		C	3.308195	1.003997	0.922906
		C	2.627816	2.283698	1.340503
		H	3.352316	3.107843	1.394730
		H	2.150329	2.188847	2.328891
		H	1.836421	2.564783	0.627710
		C	-2.391676	-0.200922	0.922506
		C	-3.079678	1.029317	1.007804
		C	-2.432258	2.290479	1.525310
		H	-2.866593	3.176957	1.042926
		H	-1.352868	2.316440	1.339442
		H	-2.607074	2.388405	2.611293
		C	-4.442481	1.049167	0.671064
		H	-4.974639	2.004510	0.707684
		C	-5.137597	-0.109870	0.310103
		C	-6.591318	-0.052675	-0.094290
		H	-7.140852	-0.942279	0.248108
		H	-6.689203	-0.011269	-1.191979
		H	-7.088932	0.838613	0.314373

Table S2. %V<sub>Bur</sub> values (by quadrants) for (a) Rh-Id and (b) Ru-I.

	Quadrant	V <sub>f</sub>	V <sub>b</sub>	V <sub>t</sub>	%V <sub>f</sub>	%V <sub>Bur</sub>
(a)	SE	30.6	14.3	44.9	68.1	31.9
	NE	30.6	14.3	44.9	68.1	31.9
	NW	33.0	11.8	44.8	73.7	26.3
	SW	30.0	14.9	44.9	66.9	33.1
(b)	SE	30.7	14.1	44.9	68.5	31.5
	NE	31.0	13.8	44.9	69.1	30.9
	NW	32.5	12.3	44.8	72.6	27.4
	SW	29.8	15.0	44.9	66.5	33.5



**Figure S1.** Topographic steric maps of the NHC ligands for the studied complexes (a) **Rh-Id** and (b) **Ru-I**. %Vbur is the percent of buried volume. The metal is at the origin and the P atom is on the z axis. The isocontour curves of the steric maps are in Å.