

Kinetics of Phosphine Substitution in $\text{CpRu}(\text{PPh}_3)_2\text{X}$ ($\text{X} = \text{Cl, Br, I, N}_3$, and NCO)

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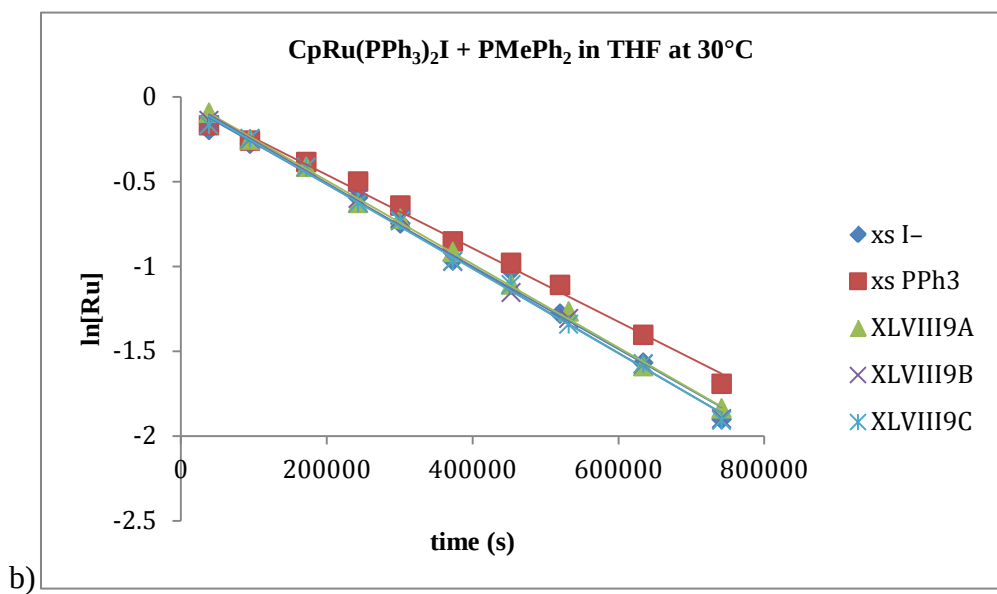
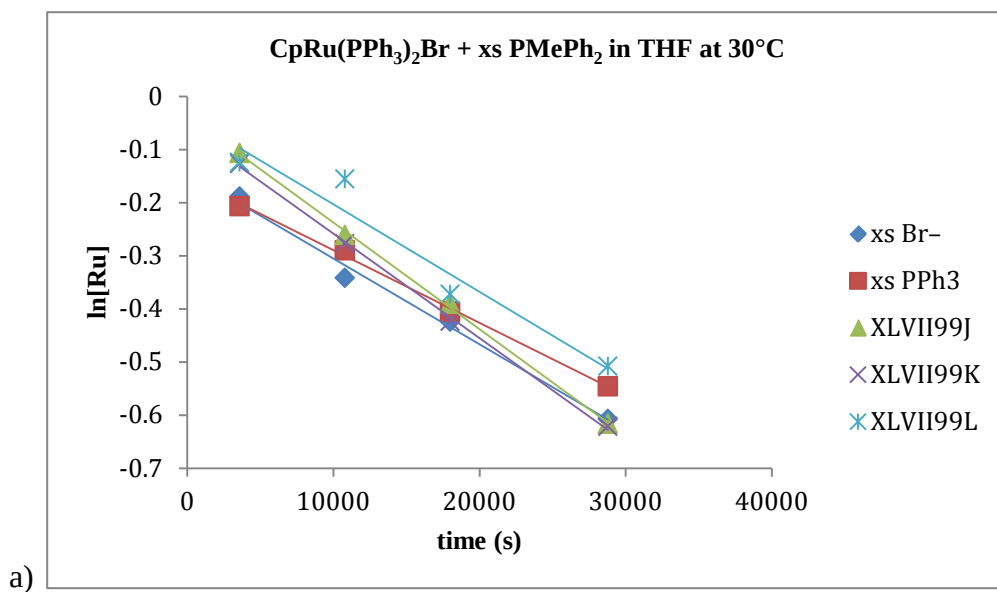
Figure S5: Plots of $\ln[\text{CpRu}(\text{PPh}_3)_2\text{X}]$ vs time for halide exchange in CDCl_3 at 30°C in the presence of duroquinone (DQ), 9, 10-dihydroanthracene (DHA) and PPh_3 **1c-1d** S9

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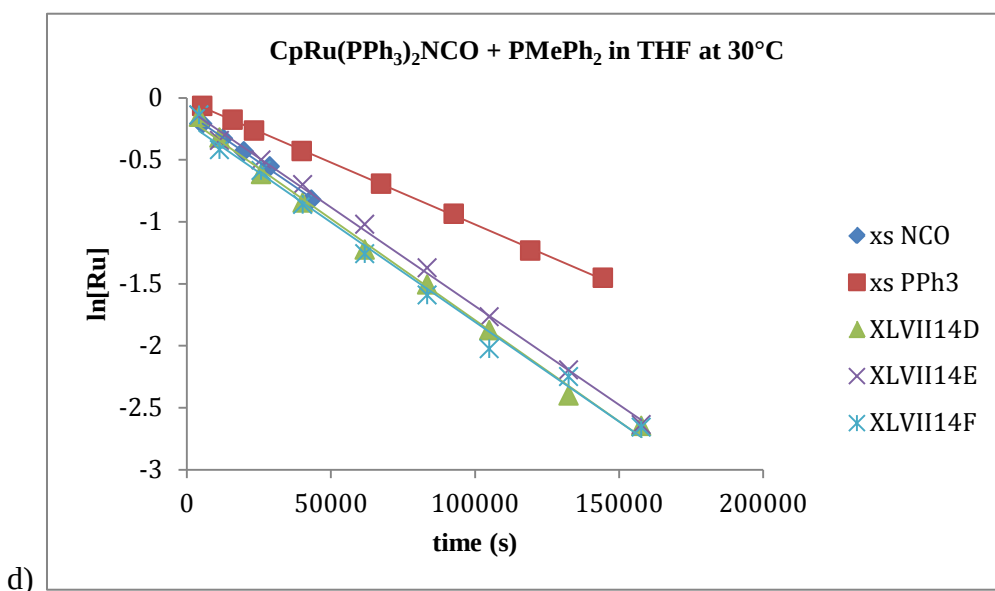
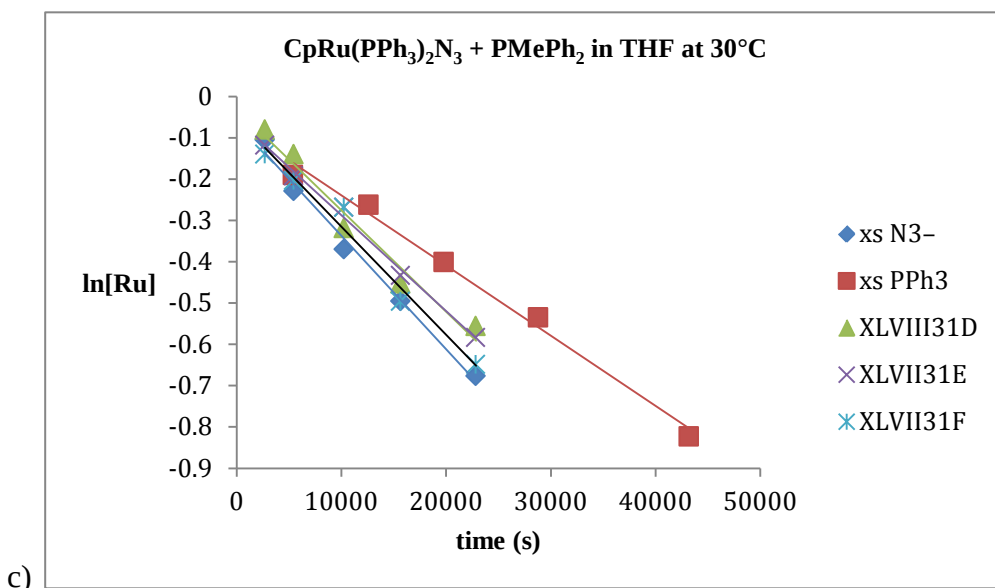
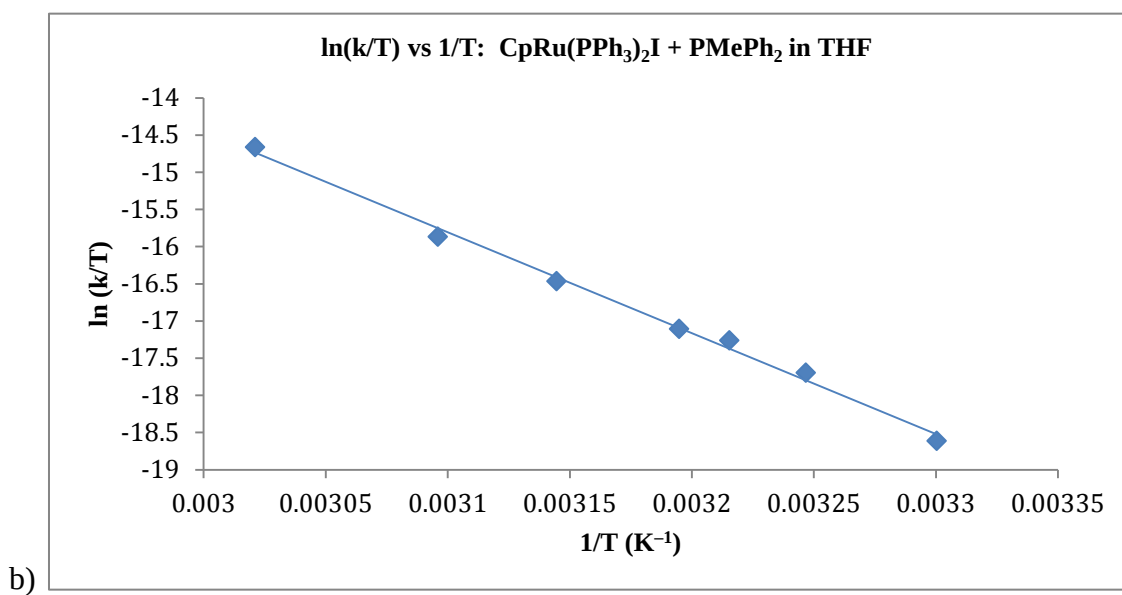
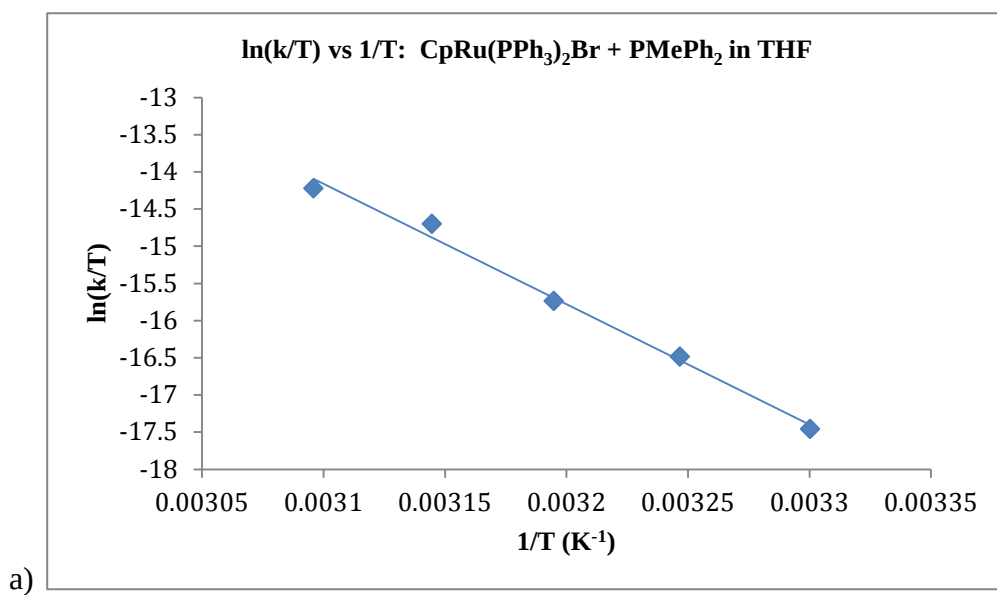


Figure S1: Plots of $\ln[\text{CpRu}(\text{PPh}_3)_2\text{X}]$ vs time for the reaction between $\text{CpRu}(\text{PPh}_3)_2\text{X}$ and excess PMePh_2 in THF at 30°C. a) X = Br, **1b**, b) X = I, **1c**, c) X = N₃, **1d** and d) X = NCO, **1e** including the effect of added X⁻ and PPh₃.



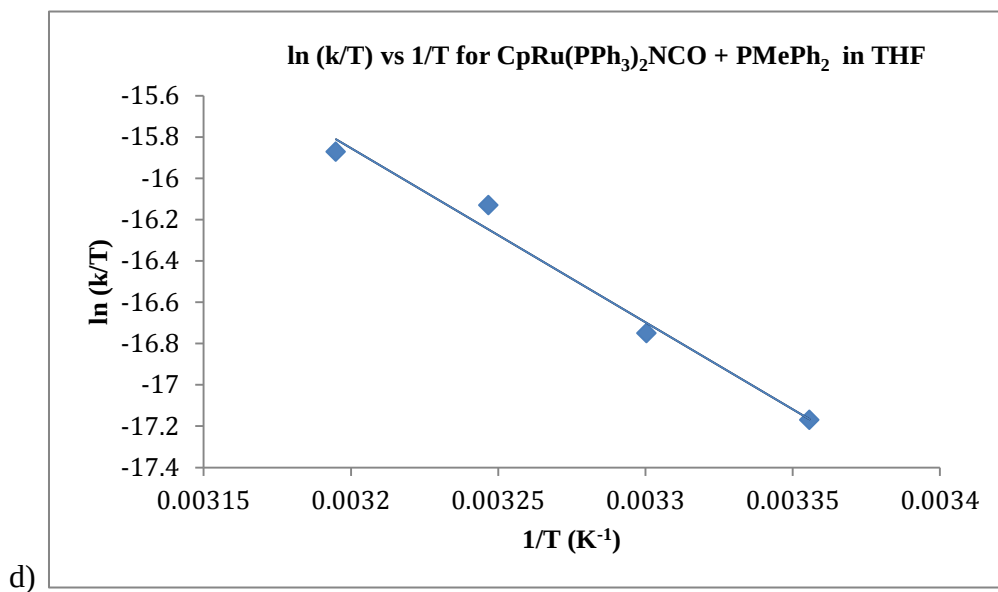
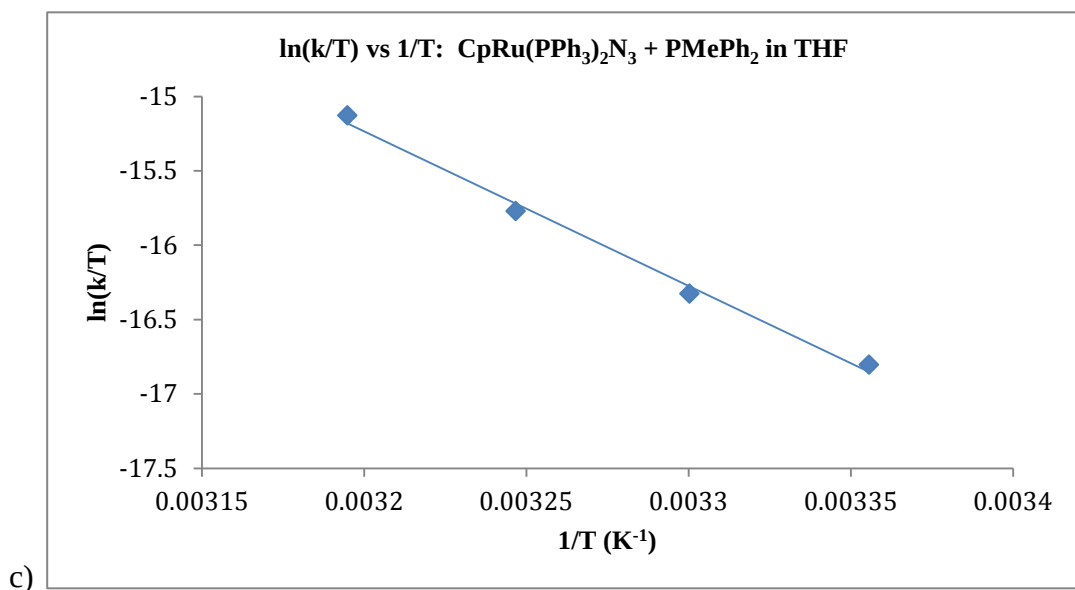


Figure S2 Eyring plots for reaction between CpRu(PPh₃)₂X and excess PMePh₂ in THF between 25 and 50°C. a) X = Br, **1b**, b) X = I, **1c**, c) X = N₃, **1d**, and d) X = NCO, **1e**.

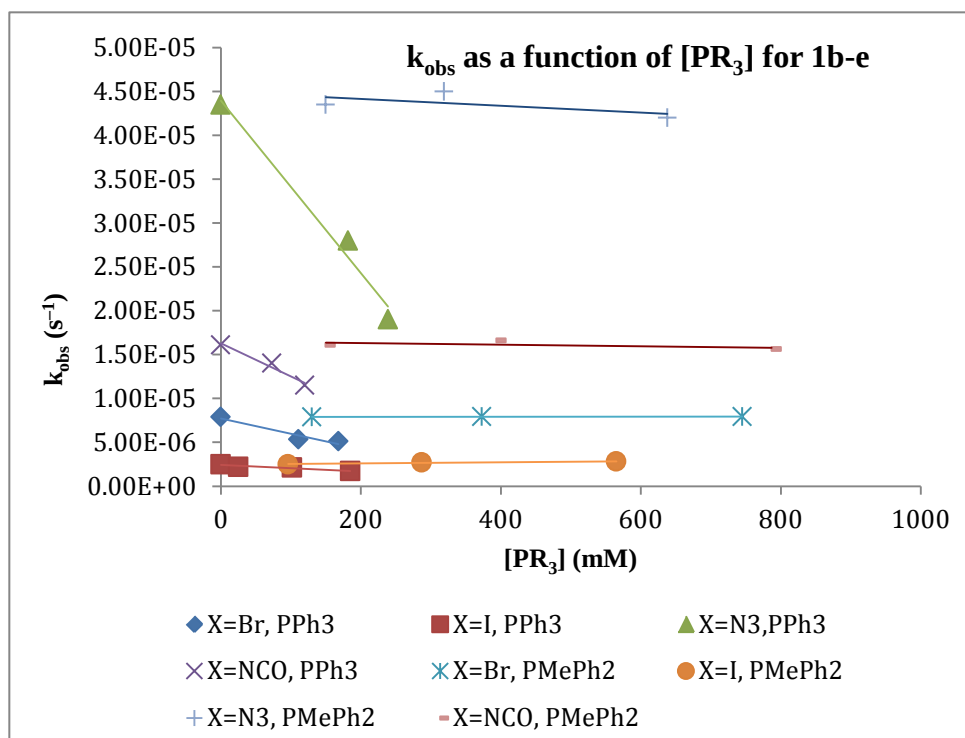


Figure S3 Plots of k_{obs} as a function of $[\text{PMePh}_2]$ and $[\text{PPh}_3]$ for the reaction between $\text{CpRu}(\text{PPh}_3)_2\text{X}$ and excess PMePh_2 in THF. The data are for reactions at 30°C except for $\text{X} = \text{N}_3$ which is for 35°C.

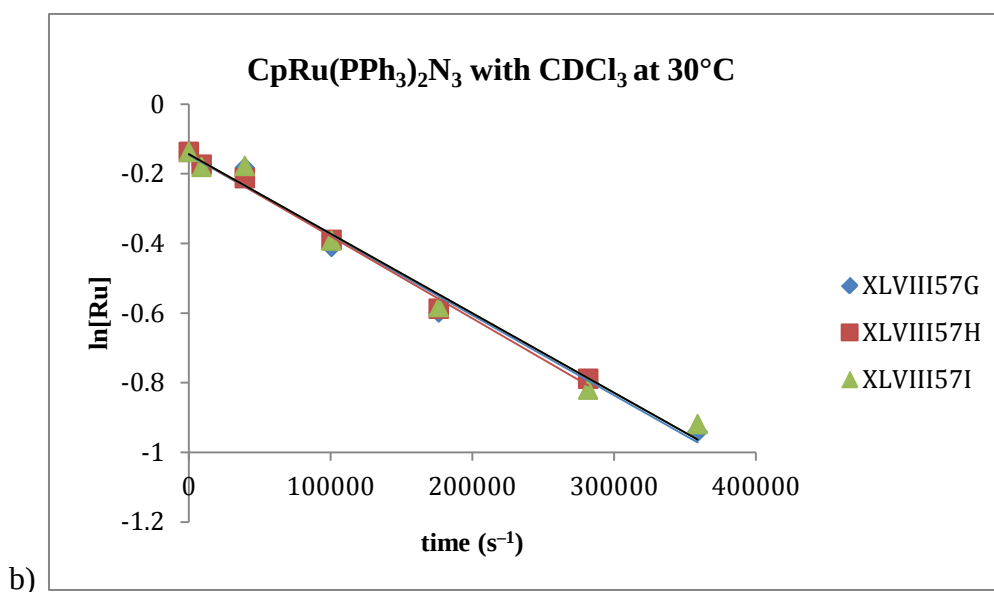
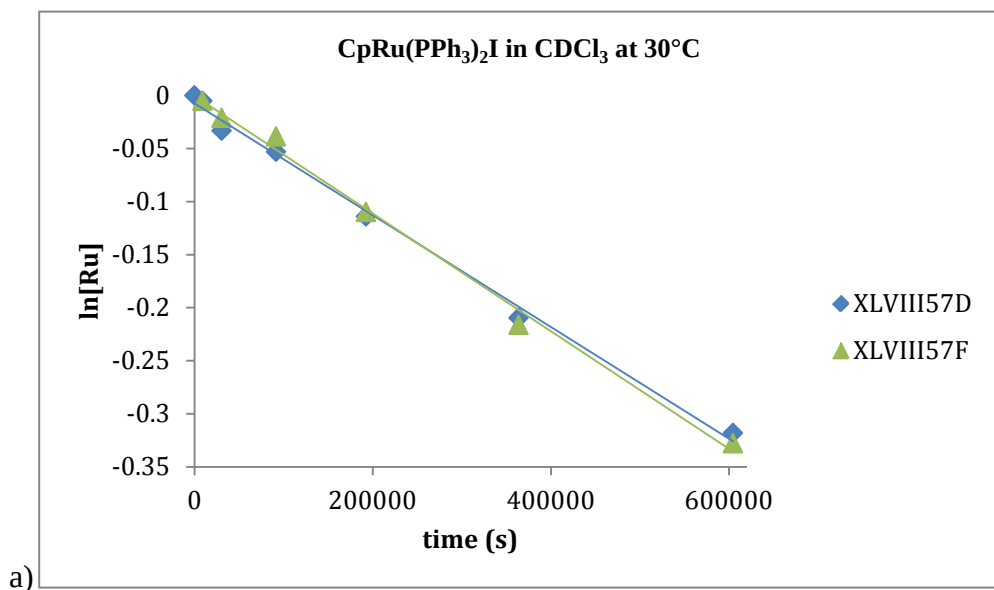


Figure S4 Plots of $\ln[\text{CpRu}(\text{PPh}_3)_2\text{X}]$ vs time for the reaction between $\text{CpRu}(\text{PPh}_3)_2\text{X}$ and CDCl_3 a) $\text{X} = \text{I}$, **1c** b) $\text{X} = \text{N}_3$, **1d**.

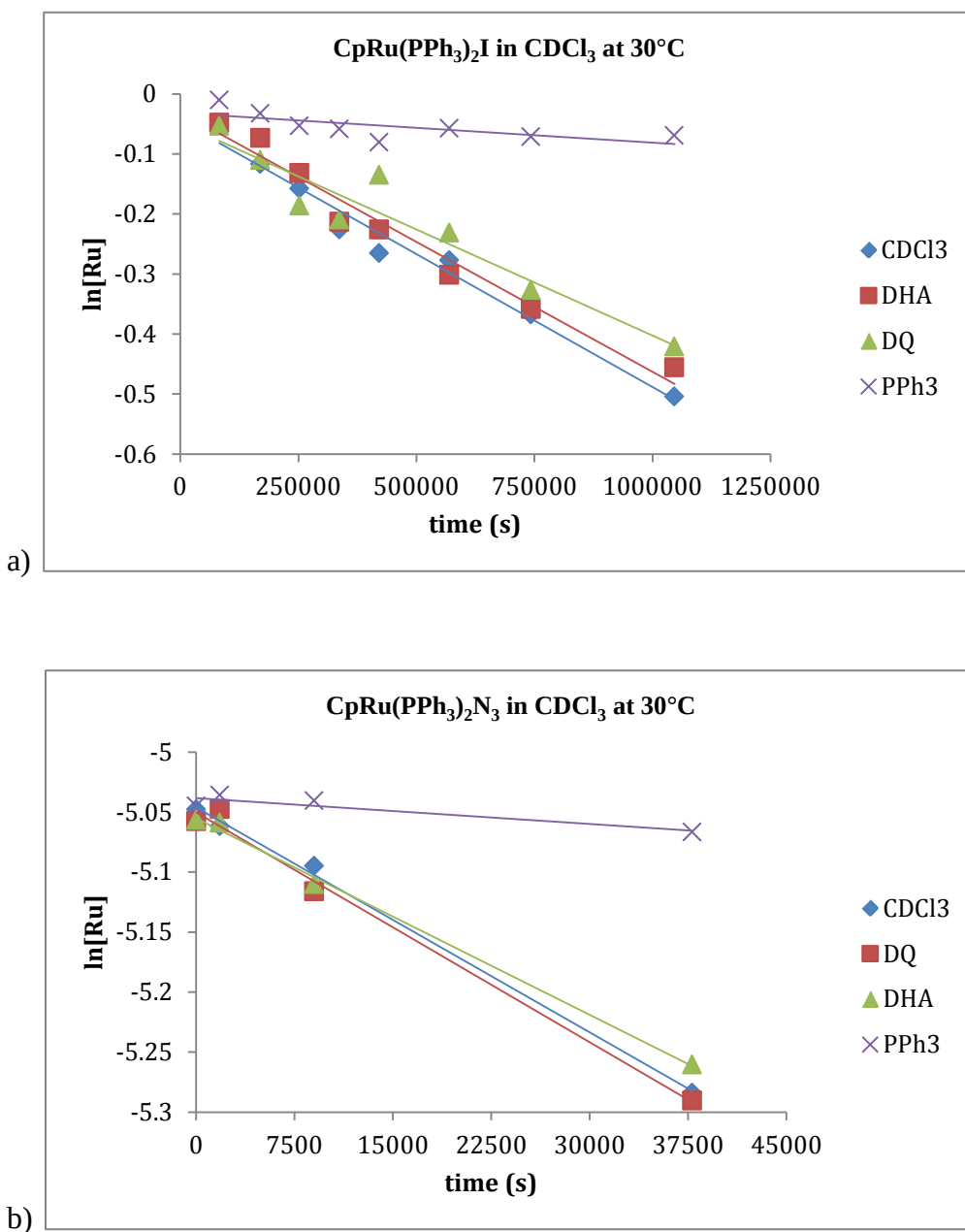


Figure S5 Plot of $\ln[\text{CpRu(PPh}_3)_2\text{I}]$ vs time (s) for halide exchange in CDCl₃ solution at 30°C. a. **1c** in the presence of 9, 10-dihydroanthracene (DHA, 3 eq), duroquinone (DQ, 7 eq) and PPh₃ (21 eq) and b. **1d** in the presence of 9, 10-dihydroanthracene (DHA, 2 eq), duroquinone (DQ, 3 eq) and PPh₃ (6 eq).

Table S1: Rate Constants for Reactions of CpRu(PPh ₃) ₂ X with excess PMePh ₂ in THF ^a								
X/k _T (x 10 ⁶)	25°C	30°C	35°C	38°C	40°C	45°C	50°C	58°C
Cl ^b		29±2			135±1		580±2	
Br		7.89±0.79	21.2±4.5		45.7±16	131±4	214±6	
I		2.49±0.03	6.33±0.03	9.88±0.15	11.6±0.8	22.4±0.5	41.3±0.5	141±5
N ₃	15.0±0.1	24.6±1.5	43.5±1.8		84.2±4			
NCO	10.2±0.2	16.1±3.6	30.4±0.4		45.7±2.1			
^a Concentrations of reactants and products were determined from integration of the resonances. Concentrations ranged from 12 to 18 mM with a $\approx$ 10 fold excess of PMePh ₂ .								
^b see <i>Organometallics</i> 1996 , 15, 302-308.								

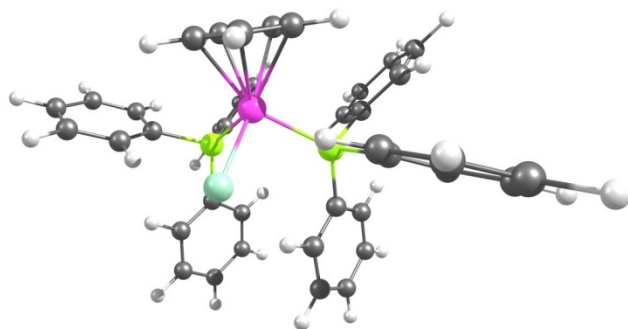
Table S2: Activation Parameters for Reactions of CpRu(PPh ₃) ₂ X with excess PMePh ₂ in THF ^a		
X	$\Delta H^\ddagger$ (kJ/mol)	$\Delta S^\ddagger$ (J/mol-K)
Cl ^b	121±4	71±8
Br	135±7	102±23
I	113±4	21±12
N ₃	86±5	-48±16
NCO	70±7	-105±23
^a from plots of ln(k/T) vs 1/T		
^b see <i>Organometallics</i> 1996 , 15, 302-308.		

Table S3: Rate Constants for Reactions of CpRu(PPh ₃) ₂ X with excess PMePh ₂ and excess PPh ₃ in THF ^a					
Compound	T (°C)	[PMePh ₂] (mM)	[PPh ₃] (mM)	[Ru] (mM)	k (x 10 ⁶ s ⁻¹)
1b	30	130	0	13	7.89±0.79
		373	0	12	7.9
		745	0	12	7.9
		128	111	12	5.3
		128	168	12	5.1
1c	30	96	0	9.7	2.49±0.3
		287	0	9.5	2.7
		565	0	9.5	2.8
		96	25	9.7	2.2
		96	102	9.5	2.1
1d	35	96	185	9.5	1.7
		150	0	11	43.5±1.8
		319	0	11	45
		638	0	11	42
		159	182	11	28
1e	30	159	239	11	19
		150	0	13	16.1±0.36
		394	0	13	17
		787	0	13	16
		149	73	13	14
		149	120	13	11.5
^a Concentrations of reactants and products were determined from integration of the resonances.					

Table S4 Calculated Free Energies for Dissociation of PPh ₃ from CpRu(PPh ₃) ₂ X and Reaction with PMePh ₂		
X Group	CpRu(PPh ₃)X => CpRu(PPh ₃)X + PPh ₃ ΔG (kJ/mol)	CpRu(PPh ₃) ₂ + PMePh ₂ => CpRu(PMePh ₂)(PPh ₃) + PPh ₃ ΔG (kJ/mol)
Chloride (1a)	47.067	-35.660
Bromide (1b)	33.48299665	-41.430384
Iodide (1c)	36.38417374	-47.06208069
Azide (1d)	29.0301493	-35.06092193
Isocyanate (1e)	35.85644832	-34.76424047

Table S5: Optimized Geometries for **1a-e**, **2a-e**, and CpRu(PPh₃)X

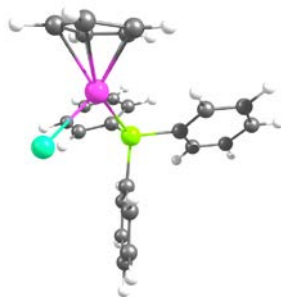
CpRu(PPh₃)₂Cl



Atomic Number	X	Y	Z
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15	1.866399	-0.006511	0.047294
15	-1.867291	0.114283	-0.019911
17	-0.042351	-0.656856	-2.824116
6	-1.055581	-3.399247	-0.711598
6	-1.110703	-3.058058	0.675005
6	0.224179	-2.970881	1.181255
6	1.11511	-3.288507	0.092607
6	0.330893	-3.538819	-1.062413
6	3.412769	-0.516914	-0.862447
6	3.336529	-1.386554	-1.959316
6	4.489791	-1.72924	-2.67709
6	5.731816	-1.207771	-2.307819
6	5.815535	-0.325154	-1.223024
6	4.664933	0.023475	-0.513885
6	1.987117	1.819441	-0.280576
6	1.611914	2.255726	-1.56443
6	1.802584	3.586745	-1.941985
6	2.355223	4.506851	-1.044755
6	2.719823	4.084011	0.23704
6	2.544777	2.747483	0.614813
6	2.358986	-0.186292	1.826872
6	1.650385	0.517823	2.81772
6	1.92974	0.331359	4.173854
6	2.912962	-0.581913	4.572422
6	3.61079	-1.303338	3.599509
6	3.338407	-1.105561	2.240747
6	-3.426369	-0.693158	-0.660856
6	-3.442223	-1.165029	-1.988587
6	-4.575733	-1.795406	-2.508851
6	-5.70781	-1.993523	-1.709852
6	-5.692626	-1.555046	-0.383766
6	-4.563941	-0.908252	0.135722
6	-1.935953	1.817324	-0.759698
6	-2.479417	2.061277	-2.0306
6	-2.512023	3.357534	-2.5555
6	-1.999522	4.431309	-1.821799

6	-1.437206	4.196072	-0.563166
6	-1.397954	2.900932	-0.042747
6	-2.33419	0.490946	1.741421
6	-3.319705	1.445787	2.062606
6	-3.686378	1.676188	3.390117
6	-3.077935	0.954818	4.425816
6	-2.096719	0.008675	4.120769
6	-1.728202	-0.216657	2.788355
1	-1.9006	-3.537696	-1.372313
1	-2.017712	-2.899597	1.245778
1	0.518781	-2.78236	2.205791
1	2.19536	-3.332583	0.147193
1	0.707057	-3.760224	-2.053352
1	2.370495	-1.761923	-2.278746
1	4.40955	-2.39608	-3.532488
1	6.6267	-1.47434	-2.865572
1	6.775081	0.098493	-0.935179
1	4.74666	0.72317	0.313778
1	1.172236	1.553757	-2.268377
1	1.507971	3.904465	-2.939142
1	2.501158	5.543199	-1.341195
1	3.154393	4.788283	0.943304
1	2.862768	2.438329	1.605512
1	0.870614	1.218843	2.534952
1	1.374342	0.898245	4.917546
1	3.130852	-0.72925	5.627537
1	4.374654	-2.019706	3.893271
1	3.902236	-1.670942	1.504791
1	-2.556135	-1.059119	-2.6096
1	-4.566018	-2.142357	-3.539793
1	-6.58611	-2.492022	-2.113506
1	-6.558369	-1.714274	0.255256
1	-4.583351	-0.585128	1.170759
1	-2.888009	1.24866	-2.619395
1	-2.943533	3.523651	-3.539894
1	-2.032839	5.439515	-2.228312
1	-1.018074	5.017072	0.013153
1	-0.954338	2.745766	0.9365
1	-3.803719	2.014293	1.273589
1	-4.449218	2.417781	3.615798
1	-3.36536	1.13415	5.459289
1	-1.610037	-0.552392	4.915246
1	-0.950133	-0.935933	2.558897

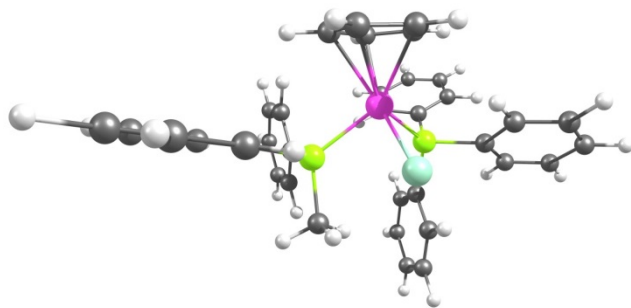
CpRu(PPh₃)Cl



Atomic Number	X	Y	Z
44	-1.901051	-0.377843	-0.163548
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6	-2.94065	1.353312	-1.033231
6	-2.593248	1.661835	0.317324
6	-3.235355	0.697073	1.165716
6	-4.059654	-0.155413	0.336727
6	-3.861336	0.235237	-1.010214
6	0.881809	1.809481	0.215172
6	0.598507	2.707817	-0.831428
6	0.809502	4.079072	-0.673227
6	1.294408	4.581588	0.541473
6	1.569385	3.699621	1.5896
6	1.367095	2.322559	1.427651
6	1.500245	-0.463326	-1.483931
6	2.591499	0.298096	-1.938644
6	3.347266	-0.127696	-3.03601
6	3.027131	-1.322171	-3.689577
6	1.946013	-2.087676	-3.23944
6	1.183502	-1.662327	-2.147443
6	1.354037	-0.8071	1.394734
6	2.753287	-0.935717	1.435142
6	3.377972	-1.540077	2.528971
6	2.61251	-2.026508	3.595901
6	1.21984	-1.911546	3.558787
6	0.593623	-1.309596	2.461801
1	-2.616705	1.888611	-1.917148
1	-1.930597	2.453348	0.64149
1	-3.162485	0.653591	2.245894
1	-4.649113	-0.997705	0.676746
1	-4.285799	-0.250977	-1.880721
1	0.21705	2.333265	-1.778651
1	0.5933	4.755681	-1.496824
1	1.945846	4.078099	2.537086
1	1.592675	1.651867	2.251503
1	2.857416	1.227412	-1.443257
1	4.186715	0.474371	-3.376379
1	1.689742	-3.018673	-3.739432
1	0.346557	-2.266481	-1.806099

1	3.360161	-0.573835	0.609764
1	4.461091	-1.636521	2.545249
1	0.617084	-2.302357	4.375014
1	-0.490441	-1.250785	2.423156
1	3.099506	-2.501339	4.444451
1	1.45506	5.649629	0.666839
1	3.614828	-1.652832	-4.54282

CpRu(PPh₃)(PPh₂Me)Cl



Atomic Number	X	Y	Z
44	0.301541	-1.152795	-0.64245
15	-1.652565	0.014303	0.067088
15	1.906883	0.0501	0.63589
17	0.066224	-2.722961	1.297453
6	1.36857	-2.608684	-2.03253
6	1.674748	-1.282198	-2.4482
6	0.461111	-0.627752	-2.841966
6	-0.601693	-1.587919	-2.695127
6	-0.050251	-2.794675	-2.189622
6	-3.184197	-1.023019	0.246402
6	-3.167331	-2.378897	-0.106665
6	-4.322512	-3.161448	0.011887
6	-5.507644	-2.598606	0.491605
6	-5.531016	-1.248233	0.864054
6	-4.378052	-0.469478	0.747171
6	-1.735165	0.923161	1.685536
6	-1.718445	0.142091	2.858194
6	-1.786334	0.748257	4.114285
6	-1.861001	2.142794	4.224381
6	-1.869441	2.924622	3.065981
6	-1.809888	2.319296	1.80373
6	-2.15768	1.285286	-1.191684
6	-1.242719	2.305551	-1.514361
6	-1.545868	3.263758	-2.484612
6	-2.76245	3.206872	-3.175482
6	-3.668094	2.184127	-2.883021
6	-3.371392	1.234097	-1.897045
6	3.59687	-0.714456	0.50219
6	3.697514	-2.102885	0.711995
6	4.944282	-2.733981	0.686032
6	6.107539	-1.994635	0.438896
6	6.015408	-0.615843	0.229594
6	4.768988	0.022022	0.26765
6	2.217425	1.820765	0.184619
6	2.160368	2.863121	1.124827
6	2.373265	4.192677	0.738465

6	2.659041	4.504257	-0.593201
6	2.719323	3.47511	-1.54154
6	2.490071	2.1525	-1.156239
1	2.073778	-3.346414	-1.673257
1	2.669144	-0.852904	-2.464471
1	0.363103	0.372178	-3.244526
1	-1.645497	-1.413418	-2.92645
1	-0.59445	-3.699306	-1.94976
1	-2.238841	-2.830423	-0.435144
1	-4.287351	-4.214663	-0.256719
1	-6.403808	-3.207291	0.588058
1	-6.445052	-0.803347	1.25082
1	-4.409197	0.573164	1.053004
1	-1.637068	-0.939509	2.786706
1	-1.775899	0.128951	5.008203
1	-1.915068	2.613296	5.20344
1	-1.932499	4.008189	3.137912
1	-1.837239	2.946387	0.918278
1	-0.279769	2.347567	-1.014667
1	-0.825352	4.047952	-2.705247
1	-2.99681	3.946393	-3.937599
1	-4.611699	2.119952	-3.420125
1	-4.093487	0.451206	-1.689575
1	2.798266	-2.684663	0.903511
1	5.005553	-3.806247	0.858206
1	7.076011	-2.488808	0.412675
1	6.912551	-0.030383	0.040826
1	4.721713	1.09643	0.116155
1	1.946157	2.652872	2.167433
1	2.318809	4.982382	1.484259
1	2.831735	5.535754	-0.890867
1	2.940329	3.70265	-2.581942
1	2.523305	1.370315	-1.908727
6	1.751031	0.10017	2.473877
1	1.601492	-0.928484	2.808587
1	2.655055	0.510709	2.933223
1	0.877407	0.679827	2.773771

CpRu(PPh₃)₂Br

Atom	X	Y	z
Ru	-0.044146099	-0.278225355	-1.370200978
P	-1.861341706	0.143280677	0.142058408
P	1.882487496	0.195413281	-0.006726756
C	0.207457507	1.329084735	-2.950147208
C	1.099870538	0.245382141	-3.277539915
C	-1.126436261	0.818589062	-3.031315303
H	0.500296937	2.353739725	-2.759848653
C	0.318721588	-0.911689298	-3.527906328
H	2.179447117	0.30506285	-3.32875636
C	-1.068287646	-0.566120259	-3.376984863
H	-2.034744134	1.384935675	-2.865154105
H	0.696350487	-1.898797318	-3.762733776
H	-1.91161823	-1.229221076	-3.51386699
C	-3.446601558	-0.42754751	-0.669660972
C	-3.522504272	-1.746852818	-1.158664454
C	-4.551825009	0.418175505	-0.866664881
C	-4.679605971	-2.210047543	-1.790860409
H	-2.666644031	-2.410447378	-1.062663774
C	-5.70432445	-0.043874847	-1.514896657
H	-4.527956809	1.447599706	-0.526472887
C	-5.77750542	-1.361344474	-1.972898167
H	-4.715028467	-3.236026004	-2.150562615
H	-6.543319069	0.633185236	-1.659330764
H	-6.674244033	-1.720494368	-2.472583438
C	-1.952749575	-0.616317107	1.835126014
C	-2.57512608	-1.851305958	2.074499014

C	-1.354748032	0.052345485	2.917950831
C	-2.621383226	-2.3889829	3.365045987
H	-3.036448633	-2.401739075	1.26321961
C	-1.408675646	-0.479537262	4.207983649
H	-0.852295726	1.003434537	2.767107213
C	-2.046022508	-1.702888187	4.438369268
H	-3.113454594	-3.345202722	3.526994237
H	-0.942487854	0.060269337	5.028385554
H	-2.089965836	-2.11841791	5.442490847
C	2.02283159	-0.099832932	1.825107289
C	2.561792208	0.824066152	2.736508765
C	1.680202443	-1.383967669	2.286003421
C	2.750152959	0.47343243	4.07871874
H	2.855804893	1.816473773	2.410050007
C	1.883596808	-1.734635594	3.622403463
H	1.255080551	-2.11131833	1.599266887
C	2.4175747	-0.809069883	4.525169469
H	3.170398217	1.201913529	4.768891012
H	1.613306394	-2.732956861	3.957633159
H	2.574107016	-1.084022167	5.565883866
C	2.374272432	1.973556076	-0.217265352
C	3.359827842	2.370185951	-1.137667158
C	1.665487152	2.977490085	0.467730463
C	3.636539637	3.724922029	-1.356287446
H	3.925911265	1.623943058	-1.687047264
C	1.949824975	4.329740519	0.261218728
H	0.881754403	2.708804718	1.169677763
C	2.938042346	4.711152919	-0.653890864
H	4.404761383	4.004973908	-2.073477589

H	1.394292988	5.083644096	0.814287035
H	3.159521085	5.763201212	-0.817014226
C	3.433845797	-0.70797908	-0.517399991
C	4.675298612	-0.374929895	0.056986858
C	3.379701271	-1.769343637	-1.431077506
C	5.83521194	-1.065347791	-0.297614171
H	4.741125174	0.426724611	0.78780645
C	4.54217449	-2.46868259	-1.78102824
H	2.423562974	-2.078645815	-1.83817684
C	5.772630158	-2.115768378	-1.222687854
H	6.78557353	-0.789746398	0.153918322
H	4.477418684	-3.297771621	-2.481853664
H	6.67464534	-2.659574697	-1.493925678
C	-2.278606673	1.912642622	0.545823037
C	-3.223624165	2.248074361	1.536031004
C	-1.686983095	2.951082696	-0.185850238
C	-3.563130777	3.580771396	1.778653355
H	-3.698770366	1.466459565	2.121705241
C	-2.029459753	4.288429804	0.050460574
H	-0.939827182	2.711133602	-0.933541309
C	-2.969388824	4.607713581	1.033150068
H	-4.294431103	3.816985766	2.548200276
H	-1.554832469	5.075545148	-0.530948957
H	-3.236329081	5.645075814	1.221450752
Br	-0.053208911	-2.828073467	-0.655523028

CpRu(PPh₃)Br

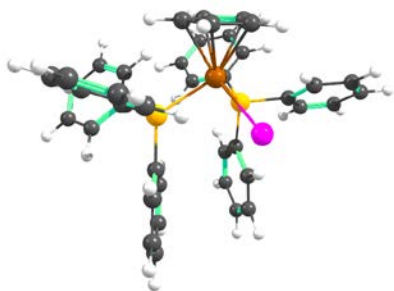
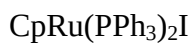
Atom	X	Y	Z
Ru	-	-	-
	0.171895389985	0.258561886857	1.390934800731
P	-	0.370240546800	-
	2.106706944679		0.064483007211
C	-	-	-
	0.351137397048	0.795222174878	3.488181394917
C	1.018254274052	-	-
		0.387501617255	3.267848917515
C	-1.200739975463	-0.338474504779	-
			3.254188373465
H	-	-	-
	0.675839924791	1.772023675217	3.826435248925
C		-0.960117784246	-
	0.997878874302		2.828228528925
H	1.891999812265	-	-
		1.022679369192	3.339536473250
C	-0.376096196951	-1.415446588262	-
			2.804332785432
H	-2.277661950968	-0.358376650037	-
			3.357584962553
H		-1.538541518671	-
	1.859692587030		2.516666409141
H	-0.708502116989	-2.411070125845	-
			2.538160030085
C	-3.649810830274	-0.226171662513	-
			0.766718023507
C	-3.725350398832	-1.575716865158	-
			1.161033511237
C	-	-	-
	4.714754284415	0.628175268461	1.090039349316
C	-4.841176559342	-2.059363933335	-
			1.846824951118
H	-2.908793627627	-2.254273180353	-
			0.924677071473
C	-	-	-
	5.830155360201	0.145142591956	1.787555631626
H	-	-	-
	4.683955186450	1.673781895241	0.798125666560
C	-5.899291975262	-1.197911326306	-
			2.165797474674
H	-4.884099398149	-3.107253759011	-
			2.134833463797
H	-	-	-
	6.645401885328	0.823060558893	2.029406627480
H	-6.766799201531	-1.572422469890	-
			2.703740281225
C	-2.052549345317	-0.651070824149	
			1.610912468676
C	-3.182189385216	-1.313819973404	
			2.123908239241
C	-0.836444819508	-0.740913040145	
			2.310749226363

C	-3.095675122406	-2.053412430939	3.307994928739
H	-4.134057472583	-1.260359399422	1.603557407884
C	-0.755381736424	-1.476126113669	3.497202362213
H	0.045310440305	-0.229869245759	1.932858700197
C	-1.881880357232	-2.137119694255	3.998290671428
H	-3.978384237155	-2.561667547760	3.689386687210
H	0.192680019452	-1.532975756764	4.026653402473
H	-1.814966419919	-2.713492910958	4.918112157691
C	-	2.053715187122	0.672772599838
C	2.569097637433	2.251787625081	1.824068337089
C	-	3.173052743212	-
C	3.349837766801	3.542660789757	0.056905275319
C	-	1.401685276588	2.227087541593
H	2.138298883487	4.464256222212	2.416594037039
H	-	0.342911378029	-
C	3.703434272295	3.035404387000	0.927189622634
C	3.675906084760	4.652208627704	1.485055698278
H	-	3.681250906790	3.123650490865
H	2.497531130256	5.321222615380	-
H	-	5.656141655081	0.229545775414
H	1.502213600448	1.802461734971	0.189369923288
C	-		
H	3.281986155303		
H	-		
H	4.303160111994		
H	-		
H	2.150845858504		
H	-		
Br	3.553978700932		
	1.379986814853		

CpRu(PPh₃)(PMePh₂)Br

atom	x	y	z
Ru	-0.090480189	-0.157412962	-1.386212772
P	-1.914680258	0.168037838	0.127768069
P	1.825413708	0.27916047	-0.018596718
C	0.092680835	1.481558669	-2.945752964
C	1.055723838	0.45966331	-3.269602103
C	-1.20614404	0.889298826	-3.059131262
H	0.318978934	2.521358421	-2.745515404
C	0.35555085	-0.742231942	-3.54319008
H	2.129369412	0.594926878	-3.307397399
C	-1.054404224	-0.484252949	-3.416914418
H	-2.151621717	1.395825278	-2.907160549
H	0.801612519	-1.702248881	-3.770220186
H	-1.852558919	-1.197083011	-3.575036987
C	-3.477250864	-0.473704865	-0.671057206
C	-3.475981931	-1.780642119	-1.196763953
C	-4.640912302	0.301124022	-0.814184816
C	-4.615304016	-2.303119791	-1.814992848
H	-2.575750041	-2.3872995	-1.134601634
C	-5.776015103	-0.21937402	-1.448440216
H	-4.676046301	1.31910626	-0.441793467
C	-5.771568005	-1.525194589	-1.944816015
H	-4.592124276	-3.318830436	-2.20356578
H	-6.662657558	0.402234702	-1.551697988
H	-6.654995389	-1.929809034	-2.433365763
C	-1.956143421	-0.607172139	1.815418153
C	-2.538033712	-1.862150428	2.05250239
C	-1.361653256	0.070303152	2.89483319
C	-2.549564621	-2.41142877	3.339089976
H	-2.994644329	-2.418655886	1.242256474
C	-1.382618069	-0.472836647	4.18112151
H	-0.887987997	1.036226823	2.744251926
C	-1.980500603	-1.716346297	4.410033554
H	-3.010064249	-3.383422689	3.500134295
H	-0.920917763	0.073756102	4.999552728
H	-1.998397803	-2.140701884	5.411281405
C	2.013067698	-0.022765791	1.807058321
C	2.554947055	0.92537811	2.691315432
C	1.695154991	-1.302430922	2.297960572
C	2.778670707	0.600139053	4.034706324

H	2.821760179	1.917261875	2.340364942
C	1.935570921	-1.628005503	3.635051002
H	1.253325178	-2.042706293	1.636108401
C	2.47761632	-0.679990917	4.50940085
H	3.201533113	1.346719416	4.703538912
H	1.685059195	-2.623388836	3.993825351
H	2.66268697	-0.935498972	5.550402291
C	2.483271269	1.998615333	-0.219149475
C	3.725353258	2.275055165	-0.813460896
C	1.694602028	3.083439393	0.206916261
C	4.165197536	3.594674448	-0.980657923
H	4.367377904	1.466554975	-1.14891629
C	2.137773254	4.399425238	0.056293539
H	0.726692258	2.90183148	0.665104695
C	3.375644473	4.661561578	-0.54427918
H	5.129105994	3.783934571	-1.447519645
H	1.514571403	5.21950763	0.405728754
H	3.719624086	5.685521091	-0.66897932
C	-2.407511536	1.915427989	0.55108156
C	-3.334515842	2.203617671	1.572116442
C	-1.887298679	2.984673596	-0.191746005
C	-3.722022647	3.5191642	1.837735867
H	-3.757420437	1.399129705	2.166535236
C	-2.278553444	4.304287775	0.066826395
H	-1.160206058	2.782330483	-0.969793947
C	-3.196767373	4.576307677	1.084184569
H	-4.436852414	3.717785158	2.632955616
H	-1.860810988	5.115649503	-0.525072335
H	-3.499954877	5.599955194	1.291357051
Br	0.066833987	-2.715009179	-0.719419956
C	3.23164982	-0.784394226	-0.596021537
H	3.414229846	-0.637037484	-1.663461983
H	4.147142166	-0.593832732	-0.027794715
H	2.925614657	-1.823107061	-0.452485779

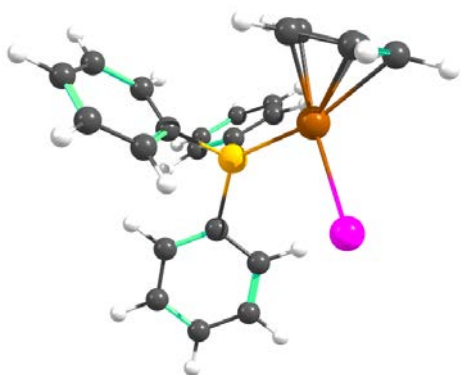


Atomic Number	X	Y	Z
44	0.022598	-0.54796	-1.21005
15	-1.89202	0.302143	-0.01072
15	1.875016	0.291342	0.095057
6	0.99489	-1.3954	-3.079
6	1.099849	0.027009	-3.1199
6	-0.21776	0.584602	-3.16108
6	-1.14612	-0.51616	-3.17341
6	-0.40467	-1.72455	-3.11468
6	-3.45883	-0.6924	-0.2139
6	-3.45925	-1.91647	-0.89571
6	-4.64047	-2.65628	-1.03643
6	-5.83756	-2.18147	-0.49669
6	-5.8468	-0.96451	0.197532
6	-4.66762	-0.23216	0.342699
6	-2.01464	0.584843	1.825379
6	-1.73594	-0.51462	2.657226
6	-1.92612	-0.42766	4.03783
6	-2.38337	0.761107	4.616844
6	-2.6512	1.863724	3.800111
6	-2.47627	1.774559	2.413692
6	-2.38599	1.937798	-0.74125
6	-1.63462	3.087702	-0.43724
6	-1.92727	4.317744	-1.03151
6	-2.96658	4.421324	-1.96372
6	-3.70928	3.28292	-2.28901
6	-3.42494	2.054368	-1.68043
6	3.467331	-0.40415	-0.60051
6	3.583853	-1.79587	-0.78051
6	4.752881	-2.356	-1.30299
6	5.824174	-1.538	-1.67924

6	5.71282	-0.15414	-1.52423
6	4.54797	0.407573	-0.98662
6	2.050739	-0.01653	1.918585
6	2.818522	-1.07289	2.432951
6	2.927523	-1.26988	3.813434
6	2.273339	-0.41324	4.703202
6	1.496982	0.635905	4.200573
6	1.379483	0.82569	2.821839
6	2.242791	2.119523	0.026011
6	3.121189	2.737542	0.937767
6	3.439127	4.092936	0.821266
6	2.895074	4.859395	-0.21663
6	2.025653	4.257923	-1.13017
6	1.700669	2.901895	-1.00357
1	1.816545	-2.09769	-3.04306
1	2.027685	0.585638	-3.12678
1	-0.47855	1.63121	-3.2522
1	-2.22404	-0.4348	-3.22773
1	-0.81336	-2.72632	-3.08593
1	-2.52989	-2.31446	-1.28571
1	-4.61581	-3.61021	-1.55802
1	-6.77051	-0.58975	0.632573
1	-4.69239	0.702454	0.896482
1	-1.36874	-1.44244	2.227272
1	-1.70573	-1.29124	4.660526
1	-3.01124	2.79351	4.23527
1	-2.72269	2.635318	1.80077
1	-0.81212	3.029067	0.269031
1	-1.33798	5.192872	-0.76738
1	-4.51869	3.346597	-3.01273
1	-4.02692	1.188506	-1.93892
1	2.754132	-2.44707	-0.517
1	4.819157	-3.43528	-1.42101
1	6.532035	0.497452	-1.81999
1	4.495083	1.485294	-0.87993
1	3.344648	-1.74608	1.766038
1	3.528673	-2.09465	4.188879
1	0.972438	1.305064	4.877785
1	0.769947	1.648	2.458638
1	3.565614	2.159483	1.741975
1	4.117581	4.548093	1.539149

1	1.591707	4.840774	-1.93941
1	1.00591	2.452328	-1.70307
1	2.364695	-0.56287	5.776598
1	-2.53073	0.827353	5.692494
1	-6.75413	-2.75702	-0.60382
1	-3.19375	5.377315	-2.42949
1	3.145954	5.913574	-0.30881
1	6.730849	-1.97345	-2.09289
53	0.059397	-3.0036	0.222195

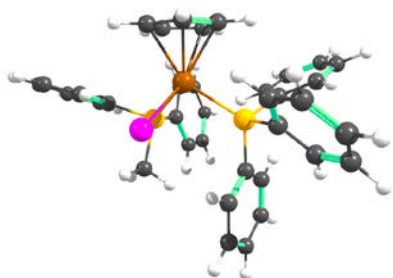
CpRu(PPh₃)I



Atomic Number	X	Y	Z
44	-1.3812	-0.85012	-0.37438
15	0.848224	0.040526	-0.01932
53	-2.75024	1.462588	-0.12769
6	-1.59696	-2.63607	0.8377
6	-0.79288	-2.98856	-0.29837
6	-1.57321	-2.75048	-1.47239
6	-2.89606	-2.33313	-1.0592
6	-2.91104	-2.26818	0.356523
6	1.336672	-0.5219	1.673391
6	0.629046	0.009837	2.769165
6	0.891404	-0.43376	4.066709
6	1.850833	-1.43002	4.291619
6	2.544478	-1.97572	3.208449
6	2.290607	-1.52425	1.906461
6	1.242549	1.848477	-0.0168
6	2.062014	2.461108	0.9449
6	2.371873	3.822151	0.849333
6	1.872136	4.584629	-0.21094
6	1.053428	3.981163	-1.17188
6	0.735179	2.62467	-1.07179
6	2.185043	-0.58987	-1.13933
6	3.535045	-0.24421	-0.94373
6	4.520514	-0.70077	-1.8213
6	4.172388	-1.49882	-2.91874
6	2.832623	-1.83277	-3.13277
6	1.84679	-1.38006	-2.24737
1	-1.29034	-2.6881	1.875378
1	0.231525	-3.33783	-0.26891

1	-1.2567	-2.91126	-2.49605
1	-3.71273	-2.06593	-1.71824
1	-3.73924	-1.93437	0.969041
1	-0.13272	0.768546	2.605398
1	0.341349	-0.00594	4.901525
1	3.287519	-2.75304	3.371279
1	2.841884	-1.95909	1.077782
1	2.459079	1.885011	1.775914
1	3.003711	4.28379	1.604717
1	0.648188	4.568807	-1.99193
1	0.077069	2.174475	-1.80964
1	3.821417	0.389922	-0.10906
1	5.559423	-0.42636	-1.65406
1	2.551002	-2.43963	-3.99014
1	0.803931	-1.62553	-2.42385
1	4.940053	-1.84817	-3.60509
1	2.051015	-1.77882	5.301867
1	2.112156	5.642784	-0.28376

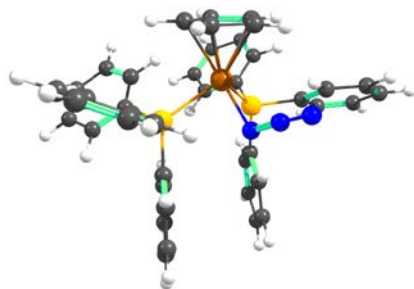
CpRu(PPh₃)(PPh₂Me)I



Atomic Number	X	Y	Z
44	0.319041	-0.73106	-0.91364
15	-1.65333	0.273497	0.00386
15	1.913717	0.249371	0.565453
53	0.100935	-3.01717	0.741753
6	1.384127	-1.86403	-2.58003
6	1.712658	-0.4851	-2.69199
6	0.510886	0.258281	-2.94015
6	-0.56476	-0.69403	-3.01852
6	-0.03609	-1.99092	-2.78612
6	-3.20516	-0.75251	-0.03103
6	-3.25387	-1.94692	-0.76227
6	-4.43317	-2.6982	-0.82789
6	-5.58006	-2.26742	-0.15643
6	-5.54037	-1.08167	0.587565
6	-4.36303	-0.33304	0.651105
6	-1.74335	0.884073	1.757493
6	-1.72392	-0.08498	2.779871
6	-1.79873	0.295283	4.121547
6	-1.88571	1.649388	4.469331
6	-1.90335	2.617508	3.461544
6	-1.83598	2.238158	2.114423
6	-2.15326	1.759492	-1.00241
6	-1.23802	2.819408	-1.14305
6	-1.54751	3.939174	-1.91916
6	-2.77167	4.012751	-2.59462
6	-3.68017	2.957576	-2.4805
6	-3.37664	1.84323	-1.68778
6	3.652141	-0.36169	0.286341
6	3.851747	-1.73949	0.086349
6	5.14225	-2.25967	-0.05107
6	6.255313	-1.41339	0.000898

6	6.067834	-0.04327	0.206696
6	4.777176	0.477811	0.35525
6	2.120287	2.08909	0.427085
6	1.84024	2.95639	1.496007
6	1.957989	4.344484	1.346651
6	2.366057	4.892125	0.128067
6	2.651097	4.039077	-0.94606
6	2.520881	2.656894	-0.79815
1	2.074322	-2.6753	-2.39076
1	2.712289	-0.07789	-2.60353
1	0.430712	1.323071	-3.11462
1	-1.6022	-0.45651	-3.21955
1	-0.59133	-2.91986	-2.76635
1	-2.35915	-2.31036	-1.25331
1	-4.44646	-3.62836	-1.39097
1	-6.42419	-0.74102	1.122066
1	-4.34928	0.581441	1.237744
1	-1.64201	-1.139	2.526919
1	-1.78498	-0.46887	4.895111
1	-1.98012	3.672053	3.717193
1	-1.87359	3.007713	1.350566
1	-0.2714	2.769445	-0.65236
1	-0.82535	4.748228	-2.00065
1	-4.63126	2.995817	-3.00673
1	-4.10208	1.039781	-1.61401
1	2.996708	-2.40981	0.058439
1	5.275084	-3.3293	-0.19661
1	7.258337	-1.81824	-0.1124
1	6.925032	0.624464	0.256615
1	4.657266	1.543497	0.525843
1	1.522885	2.562927	2.455937
1	1.732553	4.994244	2.189121
1	2.463453	5.969165	0.014589
1	2.974312	4.449926	-1.89987
1	2.746246	2.016325	-1.64568
6	1.809246	-0.01309	2.391421
1	1.827886	-1.09093	2.565361
1	2.65927	0.452845	2.89885
1	0.871695	0.37397	2.791988
1	-6.49452	-2.8544	-0.20124
1	-3.01029	4.879175	-3.20714

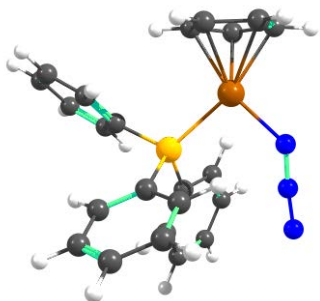
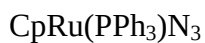
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Atomic Number	X	Y	Z
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15	-1.8565	0.135595	-0.06629
15	1.876939	0.11834	0.082005
6	1.039234	-2.7439	-2.06253
6	1.113458	-1.4887	-2.74551
6	-0.2115	-1.04228	-3.03729
6	-1.11789	-2.04557	-2.53836
6	-0.35148	-3.07936	-1.93775
6	-3.42452	-0.85419	0.131607
6	-3.37743	-2.25434	0.177533
6	-4.54007	-3.00396	0.39619
6	-5.76812	-2.36135	0.56702
6	-5.82644	-0.96189	0.531225
6	-4.66446	-0.21641	0.325574
6	-1.94986	1.060797	1.53948
6	-1.52929	0.368756	2.689402
6	-1.703	0.933578	3.954867
6	-2.28377	2.198935	4.092635
6	-2.69031	2.899287	2.952685
6	-2.5311	2.331603	1.683298
6	-2.30967	1.38863	-1.35317
6	-1.57199	2.582932	-1.44718
6	-1.81988	3.504214	-2.4676
6	-2.7995	3.241044	-3.43238
6	-3.52637	2.049008	-3.36258
6	-3.28605	1.133114	-2.33157
6	3.385141	-0.97588	0.005958
6	3.326262	-2.23748	0.630861
6	4.413229	-3.11331	0.578302

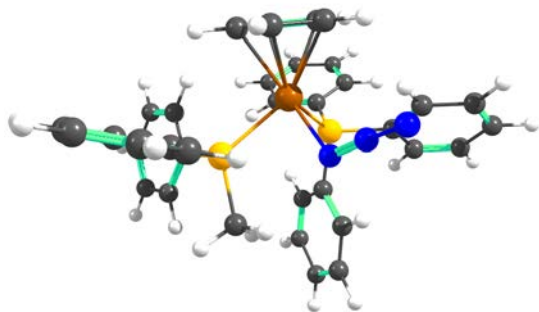
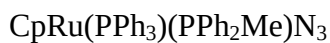
6	5.573343	-2.7601	-0.12133
6	5.63286	-1.52294	-0.76722
6	4.549884	-0.63661	-0.70204
6	1.920226	0.785054	1.816242
6	2.434743	0.053719	2.897732
6	2.446977	0.598163	4.186812
6	1.943787	1.88138	4.417191
6	1.413064	2.612465	3.34924
6	1.394018	2.065392	2.06525
6	2.423954	1.624218	-0.86146
6	3.460752	2.455093	-0.39158
6	3.875214	3.566342	-1.12816
6	3.261752	3.870959	-2.35061
6	2.227911	3.059303	-2.82306
6	1.812609	1.946496	-2.08058
1	1.876001	-3.3412	-1.72597
1	2.028346	-0.97111	-3.00755
1	-0.49096	-0.15214	-3.58628
1	-2.19759	-2.02111	-2.61492
1	-0.74214	-3.96496	-1.44979
1	-2.43036	-2.76731	0.061898
1	-4.4758	-4.08835	0.440323
1	-6.77586	-0.45063	0.673499
1	-4.72839	0.868544	0.320813
1	-1.0639	-0.60841	2.587542
1	-1.37393	0.384937	4.833899
1	-3.14384	3.883617	3.047445
1	-2.8748	2.883862	0.813761
1	-0.79392	2.801392	-0.7213
1	-1.24249	4.424891	-2.50993
1	-4.28774	1.828854	-4.1074
1	-3.8716	0.219141	-2.29318
1	2.41713	-2.53998	1.142452
1	4.345192	-4.07849	1.074918
1	6.52205	-1.23998	-1.32612
1	4.6247	0.315347	-1.21675
1	2.844569	-0.93792	2.746577
1	2.857873	0.015895	5.008384
1	1.004456	3.606266	3.514415
1	0.979293	2.653744	1.251841
1	3.944341	2.237505	0.556666

1	4.677063	4.194792	-0.74758
1	1.735954	3.290594	-3.76499
1	0.993238	1.334267	-2.4404
1	1.96075	2.306264	5.418108
1	-2.41735	2.636524	5.079422
1	-6.67207	-2.94184	0.736144
1	-2.99233	3.956081	-4.22859
1	3.585481	4.736813	-2.92356
1	6.416096	-3.4457	-0.16961
7	0.037517	-2.12138	1.202033
7	-0.2065	-3.30999	1.270436
7	-0.43776	-4.44847	1.394252



Atomic Number	X	Y	Z
44	1.898092	-0.43446	0.133461
15	-0.42048	0.147682	0.002375
7	1.592155	-2.46319	0.261706
6	3.11452	1.152501	1.075194
6	2.762305	1.580988	-0.24107
6	3.298277	0.631829	-1.17113
6	4.069122	-0.34	-0.42578
6	3.943662	-0.02822	0.948724
6	-0.74296	1.93061	-0.38098
6	-0.41927	2.901998	0.585213
6	-0.58705	4.261772	0.315177
6	-1.07168	4.677567	-0.93185
6	-1.39111	3.721204	-1.89901
6	-1.23025	2.356516	-1.62576
6	-1.405	-0.10706	1.55034
6	-2.56476	0.634399	1.841332
6	-3.28817	0.392566	3.012879
6	-2.86561	-0.5957	3.909227
6	-1.71307	-1.33625	3.629482
6	-0.98499	-1.09044	2.461329
6	-1.37345	-0.75147	-1.3047
6	-2.7403	-1.05358	-1.19503
6	-3.40387	-1.72085	-2.22883
6	-2.71206	-2.0942	-3.38591
6	-1.34852	-1.80531	-3.50064
6	-0.68289	-1.14517	-2.46368
1	2.860272	1.651927	2.00213
1	2.157293	2.442098	-0.49198
1	3.20257	0.675272	-2.24944
1	4.585972	-1.19633	-0.84124

1	4.355431	-0.60217	1.770466
1	-0.04263	2.594949	1.558367
1	-0.3391	4.996558	1.077685
1	-1.7715	4.032046	-2.86928
1	-1.49359	1.628132	-2.38707
1	-2.90277	1.410809	1.160265
1	-4.18077	0.976916	3.22413
1	-1.37551	-2.10495	4.320247
1	-0.08287	-1.66252	2.263427
1	-3.29073	-0.786	-0.2983
1	-4.46015	-1.95732	-2.12463
1	-0.79833	-2.10696	-4.38874
1	0.383356	-0.94653	-2.54691
1	-3.229	-2.61898	-4.18577
1	-1.19987	5.736236	-1.14404
1	-3.42891	-0.78335	4.820292
7	0.624296	-3.20276	0.183085
7	-0.23579	-3.9799	0.123108

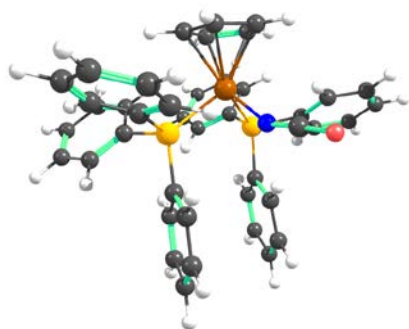


Atomic Number	X	Y	Z
44	0.270238	-1.02132	-0.69225
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15	1.914198	0.090151	0.625265
7	0.050273	-2.28795	1.089519
6	1.349959	-2.44464	-2.10586
6	1.619102	-1.10664	-2.52334
6	0.389292	-0.48361	-2.90668
6	-0.65111	-1.46434	-2.73831
6	-0.06554	-2.66008	-2.24114
6	-3.19984	-0.86702	0.233337
6	-3.20606	-2.21293	-0.15607
6	-4.35993	-2.9941	-0.01837
6	-5.52606	-2.4352	0.509293
6	-5.53012	-1.09263	0.910426
6	-4.37594	-0.3182	0.780253
6	-1.70551	1.020669	1.697235
6	-1.69169	0.205437	2.84603
6	-1.72941	0.774523	4.120375
6	-1.76889	2.166553	4.272503
6	-1.77382	2.982453	3.137887
6	-1.74587	2.413777	1.857714
6	-2.16689	1.468872	-1.16239
6	-1.24144	2.484127	-1.46969
6	-1.54434	3.473546	-2.40795
6	-2.77148	3.452724	-3.08223
6	-3.68801	2.435458	-2.80482
6	-3.39149	1.454241	-1.84979
6	3.551591	-0.77469	0.469636
6	3.588126	-2.14728	0.782047
6	4.788316	-2.85871	0.715669

6	5.969415	-2.21666	0.321834
6	5.940033	-0.85673	0.002491
6	4.739872	-0.13761	0.080511
6	2.353062	1.853958	0.266888
6	2.646137	2.783093	1.279867
6	2.989992	4.10314	0.965915
6	3.059517	4.516678	-0.36774
6	2.77051	3.601852	-1.38699
6	2.411731	2.288908	-1.06923
1	2.080455	-3.17036	-1.77238
1	2.602369	-0.65211	-2.55129
1	0.261806	0.514657	-3.3052
1	-1.70135	-1.31401	-2.95738
1	-0.58551	-3.57941	-1.9988
1	-2.3006	-2.66326	-0.54446
1	-4.33541	-4.04084	-0.31063
1	-6.43009	-0.65103	1.332351
1	-4.39092	0.716294	1.113488
1	-1.63948	-0.87511	2.741299
1	-1.72351	0.128949	4.995567
1	-1.80942	4.064502	3.242632
1	-1.77207	3.06724	0.991406
1	-0.27131	2.497237	-0.98195
1	-0.81681	4.254551	-2.6171
1	-4.64	2.40023	-3.32956
1	-4.12182	0.676339	-1.65187
1	2.672465	-2.65674	1.073484
1	4.799208	-3.9167	0.967587
1	6.902277	-2.77265	0.264863
1	6.851237	-0.34796	-0.30426
1	4.742565	0.92152	-0.1604
1	2.610031	2.488683	2.323775
1	3.207508	4.805842	1.766946
1	3.332771	5.540757	-0.61057
1	2.818273	3.910653	-2.42883
1	2.165881	1.596327	-1.86813
6	1.719223	0.058515	2.460063
1	1.378551	-0.94486	2.724791
1	2.665888	0.27065	2.964721
1	0.956383	0.77154	2.77621
1	-6.42245	-3.04093	0.620201

1	-3.00588	4.216497	-3.81996
1	-1.79893	2.608737	5.265616
7	-0.2156	-3.46271	0.923132
7	-0.47515	-4.59654	0.819899

CpRu(PPh₃)₂NCO

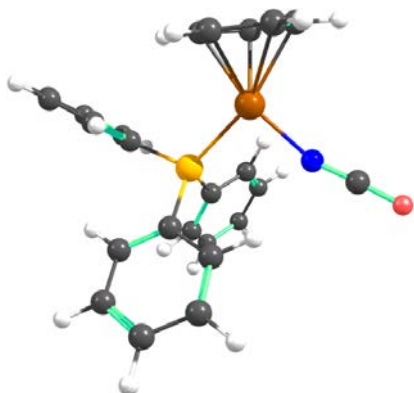


Atomic Number	X	Y	Z
44	0.030687	-0.71648	-1.22475
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15	1.867206	0.105144	0.084863
6	1.036995	-1.58301	-3.07161
6	1.095225	-0.15552	-3.14488
6	-0.23666	0.357611	-3.20966
6	-1.13031	-0.77359	-3.19679
6	-0.34955	-1.95475	-3.10454
6	-3.40841	-0.86158	-0.26506
6	-3.32545	-2.16285	-0.78011
6	-4.47278	-2.95641	-0.90276
6	-5.71799	-2.45794	-0.51284
6	-5.80992	-1.16376	0.01558
6	-4.66398	-0.37752	0.147284
6	-1.95254	0.311861	1.816819
6	-1.51206	-0.7927	2.56719
6	-1.68802	-0.82043	3.952312
6	-2.29002	0.257035	4.61084
6	-2.71649	1.365855	3.87318
6	-2.55635	1.391199	2.483091
6	-2.33971	1.818491	-0.67069
6	-1.62675	2.954864	-0.24728
6	-1.89381	4.214973	-0.7884
6	-2.86841	4.363453	-1.78224
6	-3.57022	3.238972	-2.22667
6	-3.31003	1.979391	-1.67474
6	3.401854	-0.79897	-0.47047
6	3.356104	-2.20578	-0.52578
6	4.468473	-2.94244	-0.94025
6	5.641589	-2.28916	-1.33592

6	5.687998	-0.89314	-1.31434
6	4.579604	-0.15351	-0.8823
6	1.92255	-0.07945	1.932614
6	2.404497	-1.24325	2.552638
6	2.425424	-1.35298	3.947176
6	1.963348	-0.30349	4.74637
6	1.462912	0.852429	4.138833
6	1.434191	0.958337	2.746873
6	2.36349	1.887024	-0.09692
6	3.382785	2.456828	0.692508
6	3.764296	3.788156	0.51534
6	3.135396	4.578668	-0.45569
6	2.118364	4.02793	-1.2387
6	1.735396	2.692982	-1.05631
1	1.881869	-2.25672	-3.02264
1	2.003782	0.434275	-3.16159
1	-0.52784	1.393728	-3.32701
1	-2.21063	-0.7319	-3.25369
1	-0.73098	-2.96683	-3.0447
1	-2.35792	-2.56596	-1.05674
1	-4.38556	-3.96815	-1.29164
1	-6.77254	-0.77052	0.334466
1	-4.75335	0.616845	0.576806
1	-1.03294	-1.62715	2.062784
1	-1.34523	-1.6843	4.516139
1	-3.18732	2.208743	4.374589
1	-2.91773	2.251536	1.927926
1	-0.85208	2.860789	0.508259
1	-1.33505	5.078627	-0.4353
1	-4.32707	3.338106	-3.00142
1	-3.87435	1.122498	-2.03042
1	2.437229	-2.72154	-0.26399
1	4.410595	-4.02825	-0.96322
1	6.587075	-0.37089	-1.63372
1	4.645808	0.92904	-0.88152
1	2.779343	-2.06968	1.959943
1	2.808737	-2.26205	4.40463
1	1.083225	1.670668	4.7457
1	1.03833	1.866381	2.301359
1	3.878374	1.860738	1.453566
1	4.553154	4.208277	1.134955

1	1.614359	4.633762	-1.98813
1	0.927392	2.279128	-1.64927
1	1.987182	-0.38742	5.83035
1	-2.42573	0.233653	5.689768
1	-6.60912	-3.07404	-0.60759
1	-3.07634	5.343238	-2.20552
1	3.433702	5.615386	-0.59348
1	6.504967	-2.86188	-1.66638
7	0.021156	-2.4299	0.051847
6	-0.04622	-3.60567	0.266618
8	-0.10269	-4.78507	0.534219

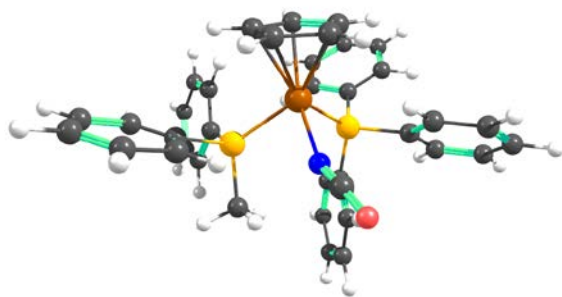
CpRu(PPh₃)NCO



Atomic Number	X	Y	Z
44	-1.82479	0.421727	-0.1847
15	0.54433	-0.02427	-0.01045
7	-2.25013	-1.58477	-0.22903
6	-2.29727	2.386508	-1.05981
6	-1.78235	2.588415	0.255004
6	-2.64601	1.903172	1.174835
6	-3.75463	1.353057	0.423844
6	-3.53199	1.636367	-0.94525
6	1.562273	1.499324	0.232327
6	1.606589	2.454575	-0.8014
6	2.301501	3.654378	-0.63644
6	2.953338	3.929771	0.57292
6	2.906164	2.993302	1.608622
6	2.217405	1.78474	1.43984
6	1.322591	-0.83234	-1.48379
6	2.617795	-0.52334	-1.93501
6	3.163139	-1.19085	-3.03679
6	2.425288	-2.179	-3.69693
6	1.1374	-2.49491	-3.25052
6	0.585694	-1.82442	-2.15507
6	1.044801	-1.12317	1.38954
6	2.300827	-1.75281	1.436262
6	2.648364	-2.5602	2.522287
6	1.744647	-2.75122	3.574731
6	0.490249	-2.13575	3.53184
6	0.140775	-1.32955	2.443046
1	-1.87099	2.766406	-1.98028
1	-0.87643	3.122118	0.510347

1	-2.52466	1.862343	2.250672
1	-4.56931	0.766195	0.830027
1	-4.15146	1.30837	-1.77161
1	1.099044	2.258038	-1.74335
1	2.331879	4.375437	-1.45001
1	3.407434	3.197014	2.55194
1	2.196975	1.066674	2.254408
1	3.206755	0.239789	-1.43416
1	4.16544	-0.93874	-3.37556
1	0.556362	-3.26228	-3.75635
1	-0.41678	-2.07226	-1.81637
1	3.008061	-1.62361	0.621577
1	3.621376	-3.0454	2.543378
1	-0.22354	-2.29314	4.336803
1	-0.84502	-0.87474	2.399636
1	2.013881	-3.38511	4.416262
1	3.491296	4.865513	0.704012
1	2.85044	-2.69782	-4.55289
6	-2.8096	-2.64497	-0.13692
8	-3.3345	-3.72248	-0.05686

CpRu(PPh₃)(PPh₂Me)NCO



Atomic Number	X	Y	Z
44	0.269426	-0.95124	-0.8159
15	-1.66088	0.165047	0.026053
15	1.909109	0.032678	0.596521
7	0.028234	-2.39752	0.740248
6	1.374123	-2.21815	-2.35131
6	1.612354	-0.84105	-2.64232
6	0.367439	-0.21283	-2.96404
6	-0.6496	-1.2309	-2.89684
6	-0.03532	-2.45153	-2.513
6	-3.21047	-0.86026	0.061009
6	-3.20217	-2.1807	-0.40716
6	-4.36515	-2.95999	-0.36857
6	-5.5516	-2.42619	0.139427
6	-5.56833	-1.11087	0.622194
6	-4.40644	-0.33809	0.590129
6	-1.72615	0.8152	1.764371
6	-1.71327	-0.14417	2.795631
6	-1.76915	0.250115	4.133567
6	-1.82794	1.609268	4.467662
6	-1.83607	2.567816	3.450754
6	-1.78928	2.174326	2.106778
6	-2.13193	1.613134	-1.03515
6	-1.22398	2.682212	-1.15396
6	-1.49902	3.76962	-1.98637
6	-2.6778	3.799004	-2.74157
6	-3.57482	2.731669	-2.65199
6	-3.30684	1.649772	-1.80365
6	3.549577	-0.80852	0.361519
6	3.584268	-2.20857	0.506959
6	4.788344	-2.90528	0.379579
6	5.97451	-2.21914	0.089328

6	5.946914	-0.83053	-0.06408
6	4.743121	-0.12743	0.07665
6	2.342977	1.824763	0.404461
6	2.633557	2.653213	1.502131
6	2.974149	3.998347	1.317594
6	3.0425	4.538521	0.030067
6	2.754502	3.725733	-1.07246
6	2.39888	2.387282	-0.8836
1	2.120087	-2.95336	-2.07975
1	2.585026	-0.36382	-2.62945
1	0.2181	0.812734	-3.27726
1	-1.70286	-1.08678	-3.10482
1	-0.53818	-3.39782	-2.35439
1	-2.27587	-2.61079	-0.76932
1	-4.33412	-3.98823	-0.72049
1	-6.48395	-0.69054	1.03192
1	-4.4312	0.674319	0.985313
1	-1.64849	-1.20038	2.549515
1	-1.76241	-0.50594	4.91515
1	-1.8886	3.625931	3.697205
1	-1.82021	2.937177	1.335613
1	-0.28796	2.663633	-0.60413
1	-0.78633	4.588773	-2.04983
1	-4.48899	2.735377	-3.24117
1	-4.02104	0.834458	-1.75084
1	2.66499	-2.75048	0.715113
1	4.79803	-3.98582	0.50307
1	6.910196	-2.76323	-0.01599
1	6.862221	-0.28766	-0.28924
1	4.746485	0.95297	-0.03396
1	2.598653	2.259457	2.512705
1	3.190614	4.620685	2.182774
1	3.313677	5.581731	-0.11326
1	2.799723	4.134219	-2.0795
1	2.150951	1.778027	-1.74708
6	1.712006	-0.16914	2.419977
1	1.390512	-1.19805	2.591177
1	2.653844	0.011358	2.945392
1	0.935518	0.497471	2.798663
1	-6.45424	-3.03176	0.173748
1	-2.88955	4.640749	-3.39666

1	-1.87081	1.916156	5.510105
6	-0.19313	-3.5133	1.115672
8	-0.40928	-4.62242	1.549047

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