

Phosphine Substitution Reactions of (η^5 -cyclopentadienyl)ruthenium

bis(triarylphosphine) chloride, $\text{CpRu}(\text{PAr}_3)_2\text{Cl}$ { $\text{PAr}_3 = \text{PPh}_3, \text{P}(\text{p-CH}_3\text{C}_6\text{H}_4)_3, \text{P}(\text{p-FC}_6\text{H}_4)_3, \text{P}(\text{p-CH}_3\text{OC}_6\text{H}_4)_3, \text{and PPh}_2(\text{p-CH}_3\text{C}_6\text{H}_4)$ }: A Tale of Two Mechanisms

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Figure S1: Cyclic Voltammograms of 1×10^{-3} M $\text{CpRu}(\text{PAr}_3)_2\text{Cl}$ in CH_2Cl_2 and 0.1 M ${}^n\text{Bu}_4\text{NPF}_6$ at a scan rate of 100mV/s

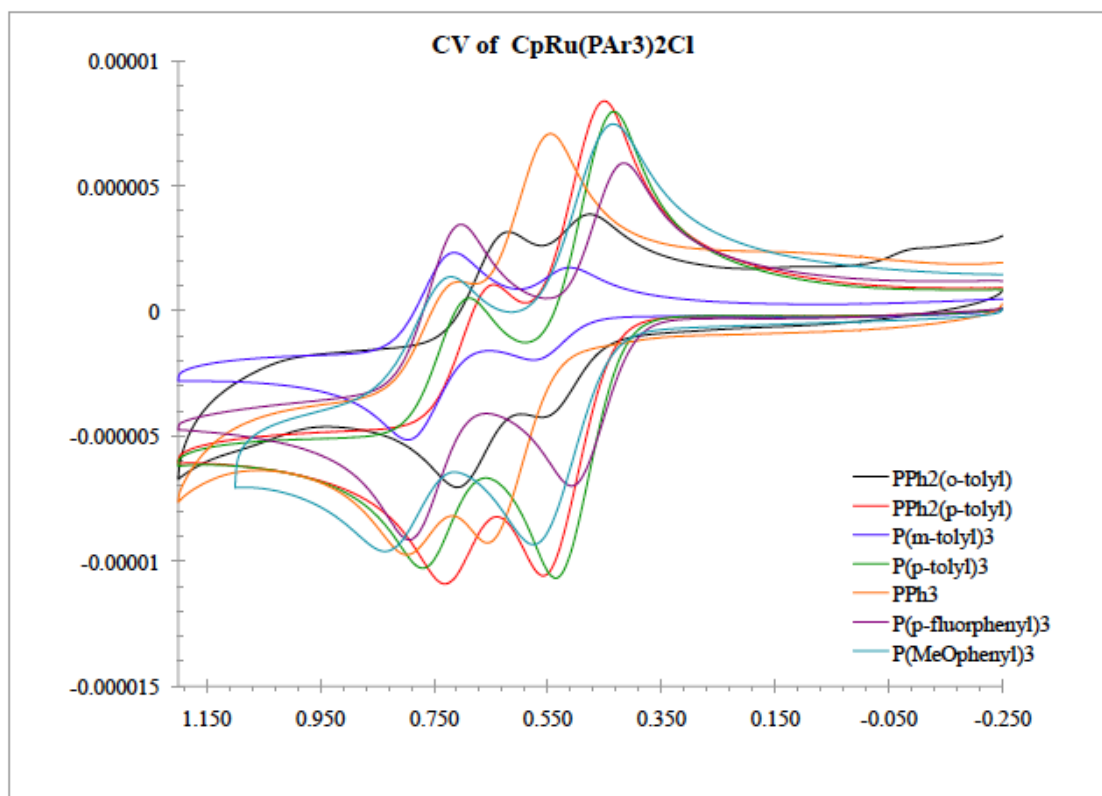


Figure S2: Representative plots $\ln[\text{CpRu}(\text{PAr}_3)_2\text{Cl}]$ vs t @ 25°C for **1a-e**

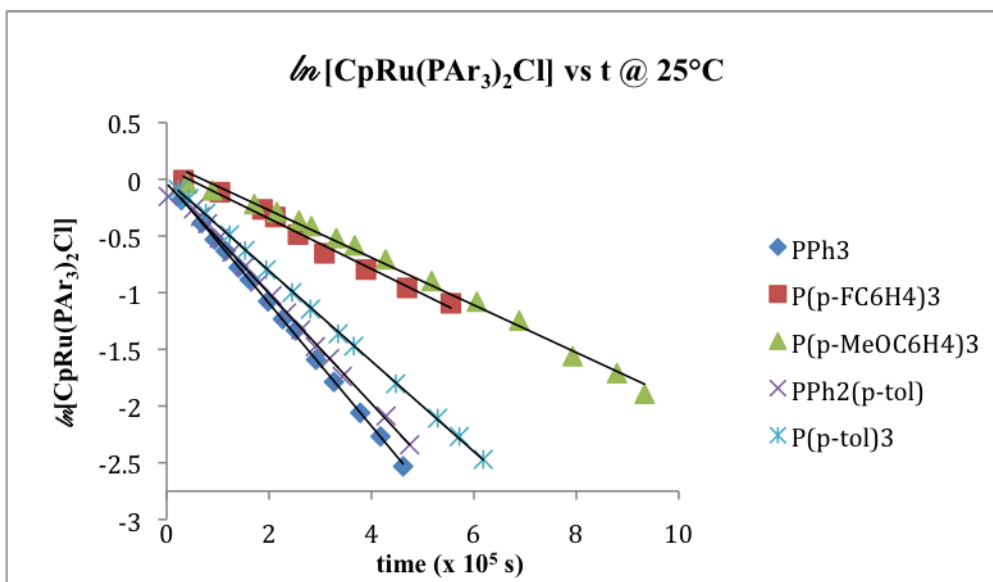


Figure S3: Arrhenius plots $\ln(k_{\text{obs}}/T)$ vs $1/T$ for **1a-e**

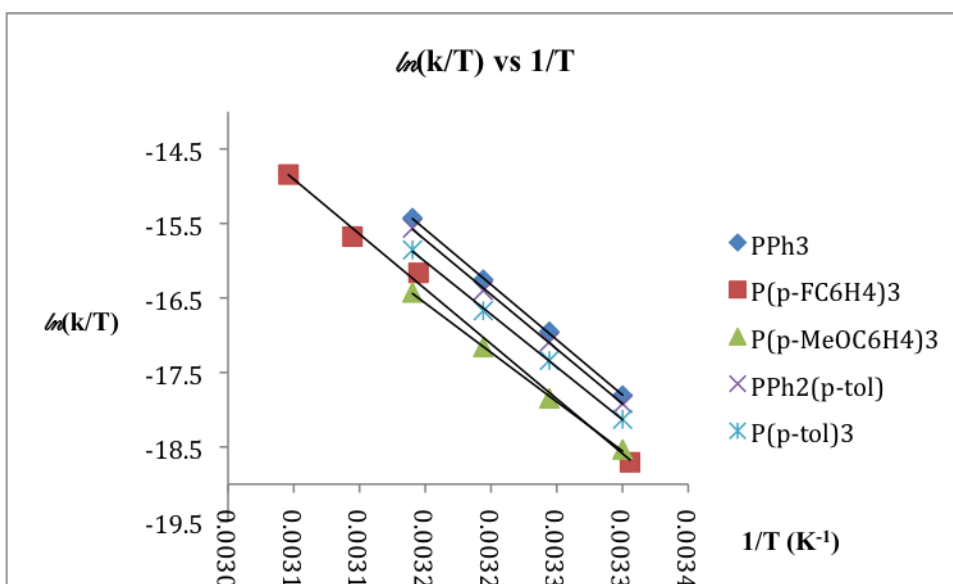


Figure S4: Plot of $\ln k_{\text{obs}}$ vs $[\text{Cl}^-]$ for **1b-d**

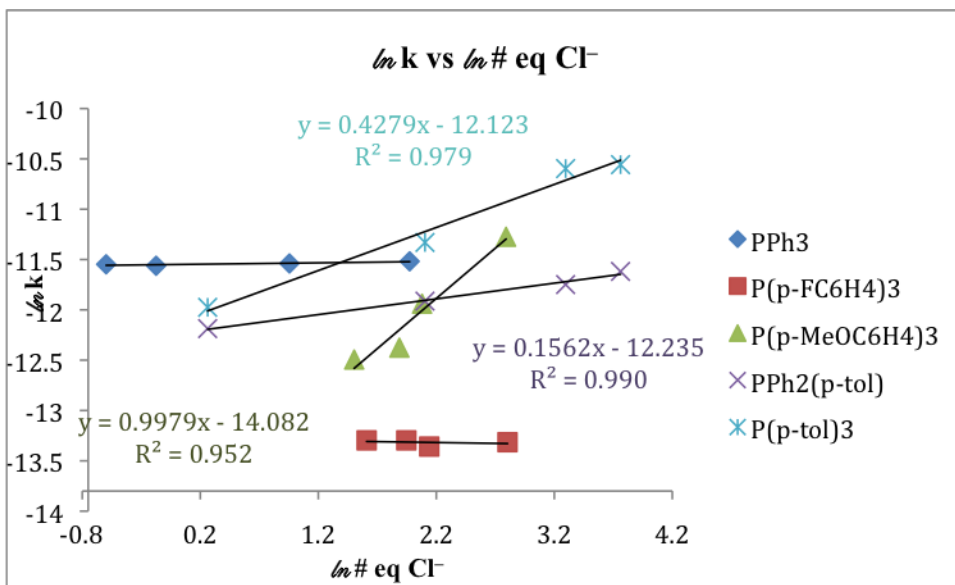


Figure S5: Plot of k_{obs} vs Hammett σ parameter for **1a, c-e**

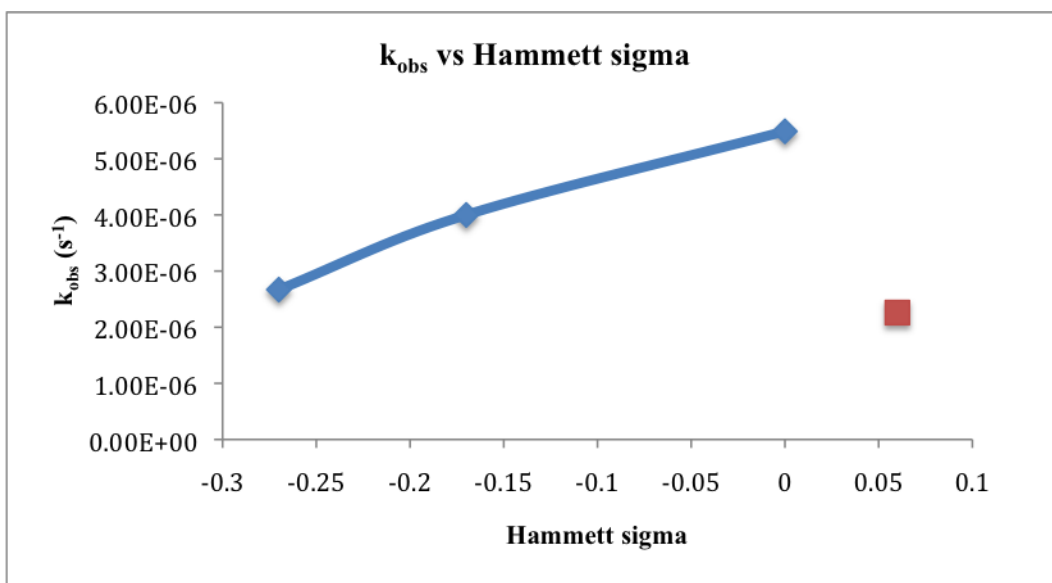


Table S1: Rate Constants, k_{obs} , ($\times 10^6$) for the reaction of **1a-e** with excess PMePh₂:

$\text{CpRu}(\text{PAr}_3)_2\text{Cl} + \text{xs PMePh}_2 \rightarrow \text{CpRu}(\text{PAr}_3)(\text{PMePh}_2)\text{Cl} + \text{PAr}_3$						
Compound/T (°C)	25.3±0.2	30.4±0.2	35.1±0.2	40.3±0.2	45±1	50±1
1a	5.491±0.06	13.16±0.09	26.86±0.74	62.44±0.74		
1b	4.770±0.04	11.35±0.24	22.77±0.10	53.42±0.83		
1c	3.996±0.02	8.956±0.04	17.72±0.29	40.75±0.74		
1d	2.665±0.04	5.378±0.01	10.88±0.44	23.02±0.05		
1e	2.26±0.05			29.9±0.2	49.5±0.7	115±7

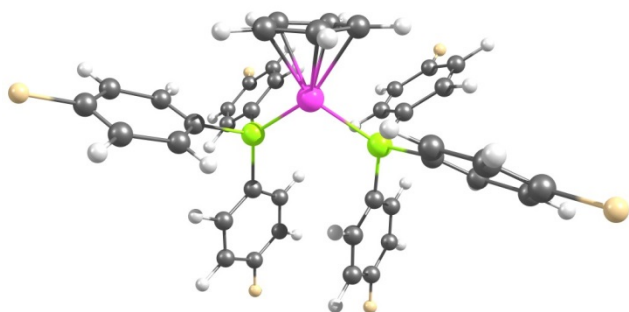
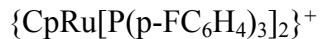
Table S2: Product ratios for the reaction of **1a-e** with excess PMePh₂ and excess ⁿBu₄NI

in CDCl₃: $\text{CpRu}(\text{PAr}_3)_2\text{Cl} + \text{xs PMePh}_2 + \text{xs Bu}_4\text{NI} \rightarrow \text{CpRu}(\text{PAr}_3)(\text{PMePh}_2)\text{Cl} +$

$\text{CpRu}(\text{PAr}_3)(\text{PMePh}_2)\text{I} + \text{PAr}_3$

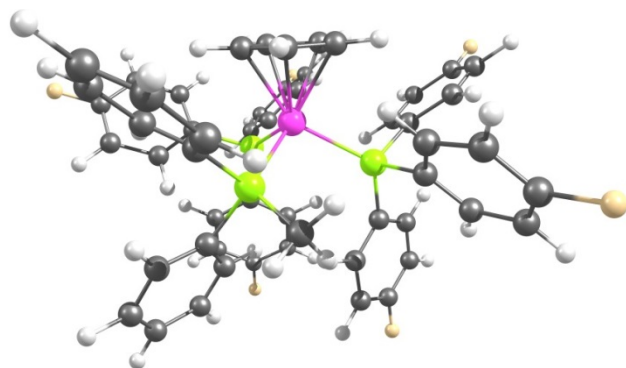
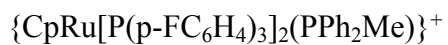
Compound	$\text{CpRu}(\text{PAr}_3)(\text{PMePh}_2)\text{Cl}$	$\text{CpRu}(\text{PAr}_3)(\text{PMePh}_2)\text{I}$
1a	32	68
1b	14	86
1c	16	84
1d	0	100
1e	0	100

Table S3: Optimized Geometries for Potential Intermediates in Figure 4



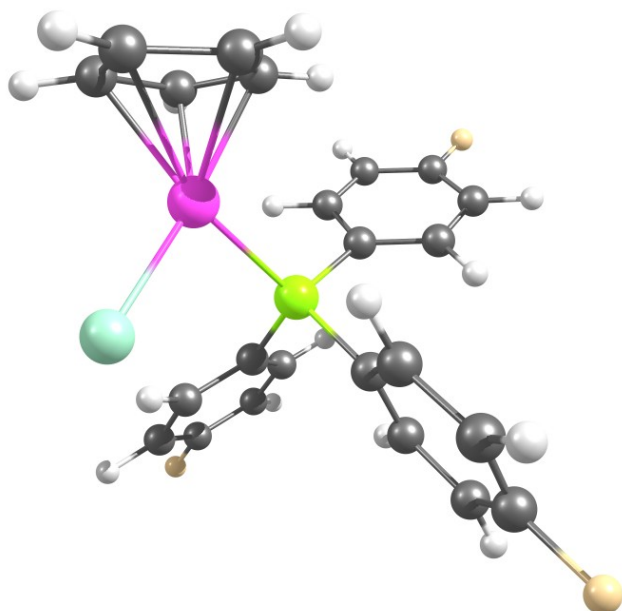
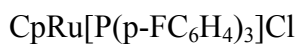
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6	0.16133	-3.30314	-0.55004
6	1.134324	-3.0625	-1.58592
6	0.429904	-2.64123	-2.74191
6	3.428857	-0.07063	-1.21052
6	3.297201	-0.3616	-2.57659
6	4.383216	-0.24771	-3.44976
6	5.608215	0.162137	-2.93288
6	5.777434	0.472206	-1.58284
6	4.680556	0.36294	-0.73051
6	1.989026	1.606704	0.53773
6	1.578603	2.610111	-0.35851
6	1.685658	3.959605	-0.02823
6	2.19769	4.297928	1.223677
6	2.606691	3.334319	2.140667
6	2.50564	1.984865	1.787153
6	2.466294	-1.17924	1.338721
6	1.666554	-1.18325	2.498365
6	1.960615	-2.01891	3.575979
6	3.059567	-2.87214	3.478275
6	3.864118	-2.90906	2.343788
6	3.561188	-2.0574	1.276352
6	-3.23369	-0.1211	-1.46998
6	-2.91055	0.30825	-2.77327
6	-3.82328	0.193584	-3.82183
6	-5.06783	-0.37937	-3.5602
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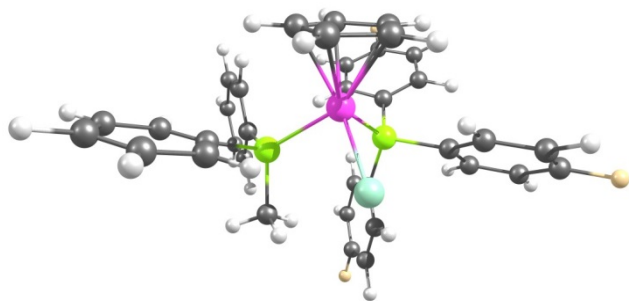
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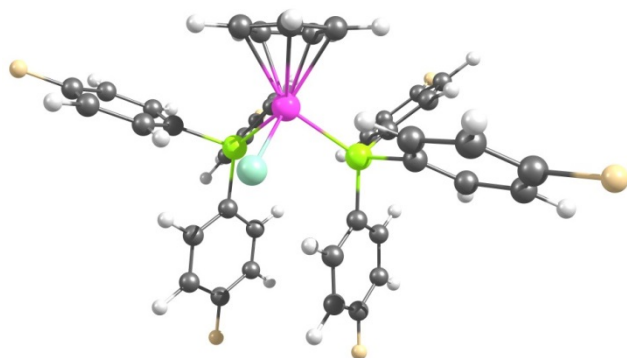
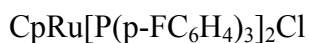
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CpRu[P(p-FC₆H₄)₃](PPh₂Me)Cl



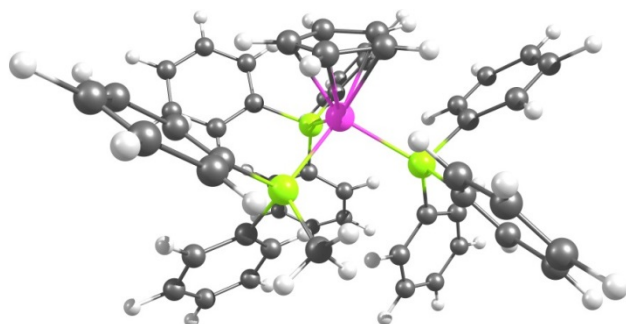
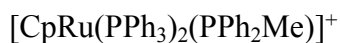
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6	1.951144	-1.197407	-2.569433
6	0.767642	-0.470922	-2.926651
6	-0.32824	-1.403749	-2.883434
6	0.1727	-2.666561	-2.472124
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6	-3.290523	2.444577	-2.795638
6	-3.029297	1.405878	-1.893664
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1	-1.770441	3.667271	3.441774
1	-1.620528	2.82049	1.113146
1	0.04349	2.38474	-0.811425
1	-0.434191	4.257569	-2.364926
1	-4.207175	2.470938	-3.37789
1	-3.767975	0.618635	-1.787032
1	2.992147	-2.904753	0.614136
1	5.175907	-4.062957	0.472152
1	7.277234	-2.75093	0.183803
1	7.168492	-0.264485	0.069907
1	5.000908	0.895624	0.241912
1	2.142691	2.305504	2.384119
1	2.540599	4.687316	1.938521
1	3.153075	5.459038	-0.350925
1	3.341632	3.791062	-2.1983
1	2.906866	1.407707	-1.765099
6	1.991264	-0.267371	2.45318
1	1.839601	-1.322847	2.686931
1	2.894472	0.094616	2.953069
1	1.118702	0.282509	2.807127
9	-6.414997	-3.302025	0.191998
9	-2.596262	4.471933	-3.803862
9	-1.773728	2.166433	5.566563



Atomic Number	X	Y	Z
44	0.469663	-0.372876	-1.284188
15	2.209902	0.049	0.358523
15	-1.482325	0.007493	0.106184
6	-0.371367	-1.037151	-3.276876
6	-0.419876	-2.105345	-2.34174
6	0.928891	-2.399864	-1.920638
6	1.819057	-1.542219	-2.662605
6	1.015589	-0.684565	-3.45487
6	2.980867	1.691229	0.0338
6	2.819906	2.284564	-1.231703
6	3.392598	3.527973	-1.518035
6	4.134212	4.196469	-0.539179
6	4.301431	3.616261	0.72392
6	3.730088	2.373413	1.009454
6	3.600206	-1.158546	0.269416
6	3.449186	-2.427288	0.858111
6	4.475804	-3.372664	0.779617
6	5.663546	-3.066777	0.105454
6	5.819581	-1.809097	-0.485017
6	4.795084	-0.858797	-0.405019
6	-3.051313	-0.489937	-0.732418
6	-3.421093	0.195148	-1.906032
6	-4.585133	-0.136793	-2.597434
6	-5.377373	-1.176157	-2.108057
6	-5.045384	-1.875578	-0.952743
6	-3.878341	-1.523034	-0.264985
6	-1.813649	1.768907	0.533306
6	-3.109224	2.212684	0.864458
6	-3.349389	3.54712	1.191087
6	-2.279661	4.441809	1.175919
6	-0.987569	4.045281	0.84307
6	-0.764756	2.703981	0.521883
6	-1.520273	-0.9138	1.701896
6	-1.971883	-0.346339	2.904683
6	-1.983916	-1.089029	4.089105
6	-1.547704	-2.410574	4.055255
6	-1.092841	-3.009592	2.880844
6	-1.074229	-2.24872	1.710885

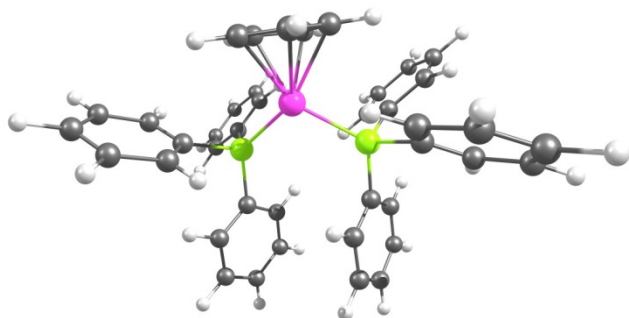
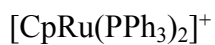
1	-1.216466	-0.585855	-3.779814
1	-1.317322	-2.601189	-1.993549
1	1.230292	-3.186693	-1.240663
1	2.899244	-1.537874	-2.599275
1	1.381954	0.11152	-4.093906
1	2.251253	1.768752	-2.003859
1	3.260093	3.971974	-2.501276
1	4.581083	5.162587	-0.758289
1	4.88066	4.129587	1.48697
1	3.883683	1.93988	1.993205
1	2.537074	-2.684035	1.392398
1	4.349788	-4.345269	1.248546
1	6.462272	-3.80127	0.046448
1	6.742392	-1.56045	-1.002866
1	4.940052	0.118129	-0.857791
1	-2.807579	1.012509	-2.277919
1	-4.885844	0.39384	-3.496179
1	-5.693436	-2.671535	-0.597804
1	-3.630925	-2.058407	0.646255
1	-3.943779	1.517464	0.86204
1	-4.344025	3.898896	1.448899
1	-0.182777	4.774124	0.831898
1	0.242797	2.400314	0.25424
1	-2.310533	0.684468	2.935368
1	-2.326504	-0.657712	5.02515
1	-0.761125	-4.043785	2.895927
1	-0.704036	-2.702952	0.795357
6	1.84097	0.081644	2.168302
1	2.756757	0.169392	2.758264
1	1.178426	0.920001	2.397086
1	1.33332	-0.840529	2.455575
9	-1.558709	-3.133848	5.192142
9	-6.501268	-1.506369	-2.775252
9	-2.506451	5.733057	1.485838



Atomic Number	X	Y	Z
15	1.27765	-1.995515	0.391227
6	2.338945	-1.513006	1.842891
6	1.857529	-0.567851	2.760956
6	2.55662	-0.294538	3.941835
6	3.754055	-0.958525	4.219379
6	4.245272	-1.901848	3.310079
6	3.541868	-2.183297	2.135584
6	2.471492	-2.981632	-0.636592
6	2.28135	-4.350355	-0.893125
6	3.188651	-5.066987	-1.684203
6	4.307925	-4.431251	-2.2261
6	4.512476	-3.069873	-1.972537
6	3.601263	-2.354015	-1.192575
1	0.939139	-0.028799	2.560928
1	2.165508	0.445567	4.634581
1	4.300237	-0.745437	5.134798
1	5.173753	-2.428335	3.517042
1	3.935737	-2.930754	1.454702
1	1.432632	-4.88336	-0.477405
1	3.019272	-6.125103	-1.867362
1	5.014512	-4.9889	-2.835117
1	5.381829	-2.562084	-2.383094
1	3.783944	-1.299642	-1.010304
44	-0.048792	-0.449819	-1.052991
15	-2.226527	-0.64441	0.125459
15	0.858168	1.788834	-0.274595
6	1.206235	-0.815083	-2.919313
6	0.435724	0.359894	-3.146419
6	-0.948783	0.015933	-3.11897
6	-1.033523	-1.397025	-2.90231
6	0.283864	-1.910663	-2.773592
6	-2.942528	-2.365542	0.274272
6	-2.497398	-3.416988	-0.542631
6	-3.098935	-4.679262	-0.492372
6	-4.156455	-4.917761	0.389391
6	-4.605122	-3.883339	1.217114
6	-4.007773	-2.621253	1.158344
6	-2.601109	-0.02297	1.840396
6	-1.825901	-0.510155	2.906471

6	-2.114968	-0.167976	4.228598
6	-3.187479	0.68408	4.513962
6	-3.965533	1.180222	3.464615
6	-3.681259	0.824864	2.140135
6	-3.532348	0.188577	-0.900102
6	-3.539349	1.591641	-0.999713
6	-4.493299	2.250806	-1.778425
6	-5.448947	1.517299	-2.491954
6	-5.444545	0.122685	-2.410112
6	-4.498615	-0.537418	-1.615559
6	2.607502	1.93242	-0.894313
6	3.634781	1.193386	-0.27976
6	4.954418	1.285706	-0.731486
6	5.271152	2.097005	-1.826835
6	4.256312	2.820381	-2.458267
6	2.938451	2.7456	-1.991891
6	0.975782	2.406175	1.476704
6	2.163314	2.861433	2.072682
6	2.144928	3.438337	3.347414
6	0.94154	3.576357	4.044504
6	-0.248002	3.132743	3.456041
6	-0.228839	2.554267	2.184818
6	0.108351	3.340336	-1.009102
6	0.534801	4.601942	-0.545489
6	0.038846	5.778161	-1.108994
6	-0.897576	5.725269	-2.1489
6	-1.333568	4.483283	-2.612877
6	-0.833852	3.304759	-2.044161
1	2.28436	-0.880357	-2.922315
1	0.842691	1.345584	-3.326911
1	-1.792133	0.663741	-3.311789
1	-1.951511	-1.967972	-2.896004
1	0.55384	-2.950058	-2.643027
1	-1.665775	-3.260445	-1.218624
1	-2.736688	-5.474902	-1.139102
1	-4.62378	-5.898067	0.433889
1	-5.425241	-4.055056	1.909658
1	-4.383276	-1.836684	1.80679
1	-0.996094	-1.179453	2.714336
1	-1.502602	-0.567315	5.033093
1	-3.417704	0.951434	5.542124
1	-4.809301	1.833962	3.671371
1	-4.324756	1.199863	1.352342
1	-2.805041	2.182302	-0.460752
1	-4.488343	3.336998	-1.824954
1	-6.190621	2.02852	-3.100239
1	-6.183249	-0.458962	-2.955845
1	-4.532216	-1.620272	-1.552448
1	3.417184	0.556857	0.572096
1	5.734786	0.725288	-0.22192
1	6.297036	2.168739	-2.178738
1	4.486604	3.457242	-3.30871
1	2.177571	3.343473	-2.48362

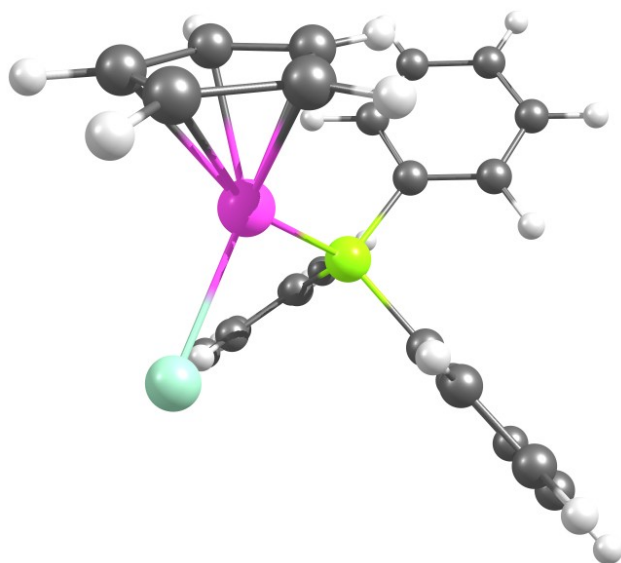
1	3.109565	2.790777	1.548744
1	3.075436	3.788375	3.787524
1	0.928548	4.032601	5.031207
1	-1.193694	3.24058	3.979974
1	-1.166482	2.23517	1.742265
1	1.259467	4.675146	0.258598
1	0.38503	6.737942	-0.733799
1	-1.282493	6.642421	-2.587366
1	-2.062662	4.423274	-3.417311
1	-1.197508	2.354905	-2.405335
6	0.353706	-3.357777	1.249162
1	-0.278045	-3.919277	0.563177
1	1.063638	-4.031284	1.737013
1	-0.294284	-2.932872	2.016059



Atomic Number	X	Y	Z
44	0.001204	-1.401366	-0.362894
15	1.967975	0.02799	-0.03299
15	-1.944862	0.101317	-0.099062
6	-0.968354	-3.37515	-0.843329
6	-1.096618	-3.117092	0.543
6	0.230097	-2.987705	1.099396
6	1.177618	-3.262482	0.048027
6	0.442167	-3.452602	-1.149051
6	3.406372	-0.426581	-1.103215
6	3.242124	-1.302092	-2.186694
6	4.312943	-1.591165	-3.04079
6	5.562185	-1.007163	-2.817895
6	5.733968	-0.122206	-1.74567
6	4.663314	0.17424	-0.901081
6	1.98595	1.858608	-0.2687
6	1.543413	2.342165	-1.512367
6	1.647738	3.69759	-1.82601
6	2.185128	4.593156	-0.893901
6	2.615275	4.123419	0.35024
6	2.52226	2.761765	0.662182
6	2.517499	-0.259275	1.703131
6	1.746035	0.266938	2.757132
6	2.084889	0.007033	4.086898
6	3.189626	-0.799621	4.387316
6	3.951651	-1.339752	3.348077
6	3.620331	-1.071357	2.01425
6	-3.204019	-0.689804	-1.197096
6	-2.88559	-0.846608	-2.561334
6	-3.769339	-1.486546	-3.43278
6	-4.979779	-2.001407	-2.951429
6	-5.295788	-1.868423	-1.597061
6	-4.416013	-1.215295	-0.723982
6	-1.990866	1.893811	-0.558823
6	-2.636708	2.383533	-1.704902
6	-2.674054	3.759519	-1.96271
6	-2.075009	4.659634	-1.078215
6	-1.427836	4.178226	0.065927
6	-1.379654	2.807524	0.319092
6	-2.700064	0.163988	1.582824

6	-3.870194	0.915528	1.805191
6	-4.441307	0.975816	3.077353
6	-3.847067	0.298447	4.149815
6	-2.675362	-0.433917	3.942939
6	-2.104831	-0.499309	2.666172
1	-1.779208	-3.489142	-1.55155
1	-2.026801	-3.006399	1.085339
1	0.478427	-2.812193	2.139082
1	2.25437	-3.290063	0.150893
1	0.860076	-3.647252	-2.129706
1	2.270966	-1.748993	-2.376422
1	4.1684	-2.266774	-3.8801
1	6.395432	-1.230942	-3.478856
1	6.70031	0.34469	-1.573374
1	4.809106	0.880651	-0.088171
1	1.128374	1.658523	-2.250695
1	1.30659	4.055124	-2.793878
1	2.268956	5.649172	-1.137289
1	3.037653	4.81229	1.077664
1	2.885223	2.41343	1.624391
1	0.880728	0.889868	2.545682
1	1.487078	0.435704	4.887421
1	3.453549	-1.002207	5.421969
1	4.811487	-1.966591	3.570305
1	4.23302	-1.493525	1.223326
1	-1.943147	-0.467176	-2.952481
1	-3.512348	-1.58637	-4.484381
1	-5.667156	-2.503491	-3.627083
1	-6.230325	-2.269578	-1.213258
1	-4.683303	-1.125083	0.324136
1	-3.13968	1.708907	-2.389549
1	-3.187984	4.123537	-2.848825
1	-2.116774	5.727997	-1.273953
1	-0.959944	4.869629	0.761414
1	-0.882187	2.455965	1.219346
1	-4.332129	1.464087	0.988736
1	-5.346296	1.557334	3.233025
1	-4.291356	0.350209	5.140399
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1	-1.182655	-1.051628	2.520096

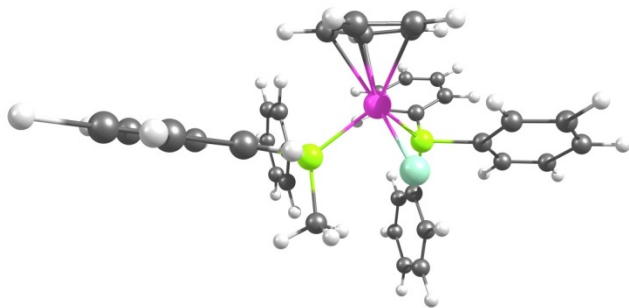
CpRu(PPh₃)Cl



Atomic Number	X	Y	Z
44	-1.901051	-0.377843	-0.163548
15	0.480894	0.016782	-0.012052
17	-1.676081	-2.760016	-0.174947
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

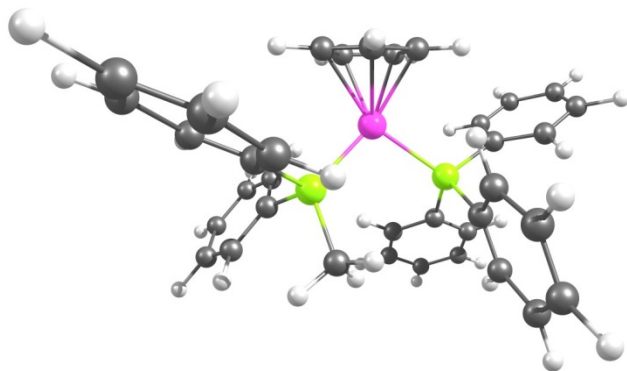
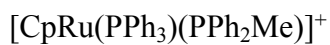
1	0.21705	2.333265	-1.778651
1	0.5933	4.755681	-1.496824
1	1.945846	4.078099	2.537086
1	1.592675	1.651867	2.251503
1	2.857416	1.227412	-1.443257
1	4.186715	0.474371	-3.376379
1	1.689742	-3.018673	-3.739432
1	0.346557	-2.266481	-1.806099
1	3.360161	-0.573835	0.609764
1	4.461091	-1.636521	2.545249
1	0.617084	-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



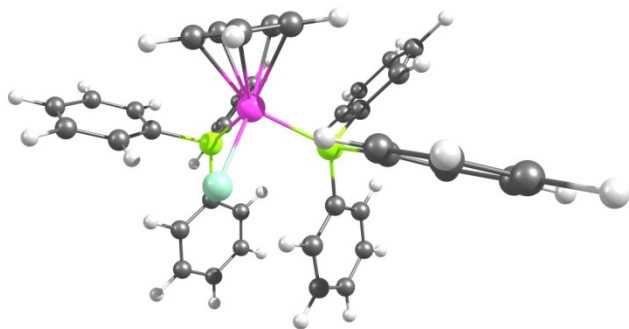
Atomic Number	X	Y	Z
44	0.301541	-1.152795	-0.64245
15	-1.652565	0.014303	0.067088
15	1.906883	0.0501	0.63589
17	0.066224	-2.722961	1.297453
6	1.36857	-2.608684	-2.03253
6	1.674748	-1.282198	-2.4482
6	0.461111	-0.627752	-2.841966
6	-0.601693	-1.587919	-2.695127
6	-0.050251	-2.794675	-2.189622
6	-3.184197	-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



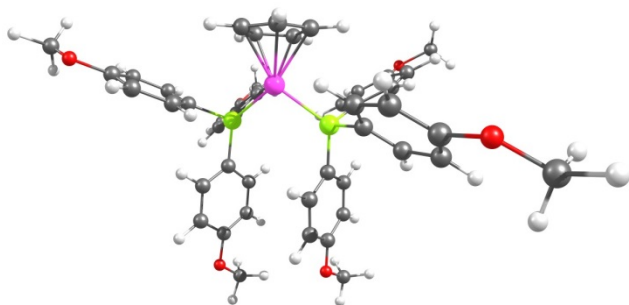
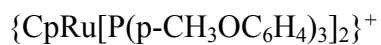
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15	-1.753619	0.057773	0.168279
6	-0.593938	-0.962153	-3.203255
6	-0.647879	-2.032873	-2.271209
6	0.69733	-2.318977	-1.832753
6	1.591927	-1.454957	-2.562861
6	0.793366	-0.600288	-3.363007
6	2.812593	1.690431	0.118305
6	2.592454	2.338417	-1.109472
6	3.243784	3.538608	-1.413399
6	4.127628	4.104917	-0.490283
6	4.357905	3.467038	0.734937
6	3.705533	2.269793	1.038318
6	3.237688	-1.178205	0.495201
6	3.006612	-2.390645	1.170106
6	3.972736	-3.401133	1.164228
6	5.178991	-3.218166	0.478665
6	5.413896	-2.017723	-0.198732
6	4.449989	-1.0032	-0.192747
6	-3.30919	-0.453284	-0.688532
6	-3.674233	0.236047	-1.860476
6	-4.829573	-0.11477	-2.560395
6	-5.633886	-1.168449	-2.106409
6	-5.278955	-1.857444	-0.944459
6	-4.124372	-1.501153	-0.23473
6	-2.097283	1.819042	0.590743
6	-3.39489	2.251491	0.924125
6	-3.633437	3.588838	1.248179
6	-2.584044	4.515886	1.235365
6	-1.29449	4.099651	0.892994
6	-1.053785	2.759347	0.572592
6	-1.793158	-0.867463	1.763008
6	-2.247776	-0.301016	2.964129
6	-2.25692	-1.055344	4.143351
6	-1.821931	-2.383865	4.136279
6	-1.367079	-2.957502	2.942587

6	-1.34386	-2.201196	1.767902
1	-1.436517	-0.512651	-3.711908
1	-1.547221	-2.532809	-1.934078
1	0.994726	-3.10207	-1.146646
1	2.671136	-1.445424	-2.486935
1	1.163183	0.19989	-3.994857
1	1.914036	1.89917	-1.839338
1	3.062656	4.027182	-2.367336
1	4.636946	5.036316	-0.723343
1	5.048004	3.900869	1.453901
1	3.908728	1.787391	1.990312
1	2.078054	-2.553218	1.712553
1	3.785132	-4.328638	1.699375
1	5.930727	-4.002957	0.477027
1	6.350983	-1.864126	-0.72785
1	4.655704	-0.071973	-0.713782
1	-3.066852	1.064922	-2.217895
1	-5.105381	0.435315	-3.456625
1	-6.532764	-1.44327	-2.651959
1	-5.902582	-2.669472	-0.579379
1	-3.876689	-2.037196	0.676366
1	-4.222875	1.547978	0.923719
1	-4.639921	3.907729	1.506538
1	-2.77372	5.556784	1.484054
1	-0.475968	4.814299	0.870293
1	-0.045356	2.458007	0.302328
1	-2.587704	0.729668	2.992907
1	-2.607512	-0.60178	5.066865
1	-1.834882	-2.967931	5.052725
1	-1.028913	-3.990713	2.927415
1	-0.972665	-2.651517	0.850423
6	1.498727	0.267522	2.272601
1	2.397552	0.363324	2.8869
1	0.862679	1.14359	2.422627
1	0.945338	-0.613661	2.601485



Atomic Number	X	Y	Z
44	-0.042464	-1.38733	-0.418936
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

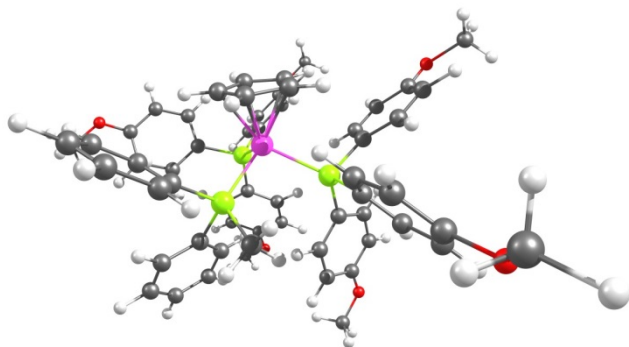
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6	-3.686378	1.676188	3.390117
6	-3.077935	0.954818	4.425816
6	-2.096719	0.008675	4.120769
6	-1.728202	-0.216657	2.788355
1	-1.9006	-3.537696	-1.372313
1	-2.017712	-2.899597	1.245778
1	0.518781	-2.78236	2.205791
1	2.19536	-3.332583	0.147193
1	0.707057	-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



Atomic Number	X	Y	Z
44	-0.192558	-1.227172	-1.230235
15	1.874795	-0.278737	-0.29758
15	-2.018679	0.07662	-0.201933
6	-1.298734	-2.66308	-2.573993
6	-1.401558	-3.098542	-1.230582
6	-0.066177	-3.334053	-0.732759
6	0.855007	-3.122239	-1.82194
6	0.100963	-2.667107	-2.932244
6	3.195108	-0.079272	-1.568082
6	2.95119	-0.346933	-2.927554
6	3.934664	-0.156213	-3.892514
6	5.207399	0.311805	-3.520609
6	5.467103	0.597028	-2.167876
6	4.464092	0.410312	-1.215208
6	2.017677	1.341533	0.570238
6	1.698049	2.505448	-0.159132
6	1.882144	3.767736	0.385313
6	2.382623	3.907538	1.693765
6	2.698772	2.762429	2.436613
6	2.519059	1.493628	1.868098
6	2.517155	-1.513815	0.907489
6	1.771588	-1.780725	2.076342
6	2.185161	-2.739154	2.992187
6	3.359062	-3.484056	2.760487
6	4.102428	-3.243537	1.596177
6	3.678079	-2.264705	0.687083
6	-3.385221	-0.041634	-1.437483
6	-3.119197	0.329486	-2.774741
6	-4.09487	0.246724	-3.75886
6	-5.381145	-0.233676	-3.441862
6	-5.657368	-0.629092	-2.125204
6	-4.664471	-0.527576	-1.141223
6	-1.91825	1.880328	0.180049
6	-2.366866	2.87726	-0.708087
6	-2.279851	4.225758	-0.378478
6	-1.746178	4.622036	0.860229
6	-1.299514	3.640307	1.759382
6	-1.378381	2.291185	1.408949
6	-2.694882	-0.597777	1.368143

6	-3.762192	0.049373	2.031186
6	-4.285267	-0.456511	3.21209
6	-3.750564	-1.629425	3.783203
6	-2.678158	-2.274592	3.149246
6	-2.165541	-1.752816	1.954989
1	-2.119824	-2.372616	-3.216805
1	-2.319222	-3.204017	-0.666144
1	0.199651	-3.699062	0.251714
1	1.928062	-3.256039	-1.783926
1	0.497978	-2.386662	-3.90079
1	1.97142	-0.695237	-3.238641
1	3.740243	-0.35549	-4.942663
1	6.433708	0.972756	-1.850091
1	4.681769	0.662698	-0.180694
1	1.315096	2.428919	-1.174493
1	1.641671	4.662617	-0.181455
1	3.093493	2.835789	3.444349
1	2.797885	0.624388	2.455681
1	0.857567	-1.227443	2.277755
1	1.618373	-2.930193	3.899365
1	5.008939	-3.799781	1.383807
1	4.27534	-2.097576	-0.204217
1	-2.131874	0.690316	-3.058335
1	-3.887609	0.545492	-4.782738
1	-6.633364	-1.012641	-1.848183
1	-4.911243	-0.84436	-0.132881
1	-2.817046	2.610239	-1.658314
1	-2.636636	4.991408	-1.061792
1	-0.885838	3.909948	2.724605
1	-1.02435	1.555453	2.126146
1	-4.180359	0.965854	1.624029
1	-5.10749	0.040682	3.719101
1	-2.234103	-3.170924	3.568677
1	-1.324897	-2.255132	1.488018
8	6.102358	0.463463	-4.530519
6	7.411608	0.954448	-4.224802
1	7.366153	1.959707	-3.790528
1	7.940197	0.277268	-3.543988
1	7.939837	0.994849	-5.177506
8	3.674903	-4.400029	3.714149
6	4.861826	-5.182622	3.548334
1	4.807328	-5.799454	2.643785
1	5.753815	-4.546666	3.512031
1	4.912973	-5.828888	4.42476
8	2.509899	5.188574	2.146844
6	3.137172	5.405288	3.414034
1	2.551728	4.968623	4.232098
1	4.153258	4.994442	3.427684
1	3.182994	6.487449	3.540306
8	-4.332293	-2.040411	4.938948
6	-3.840777	-3.223557	5.575947
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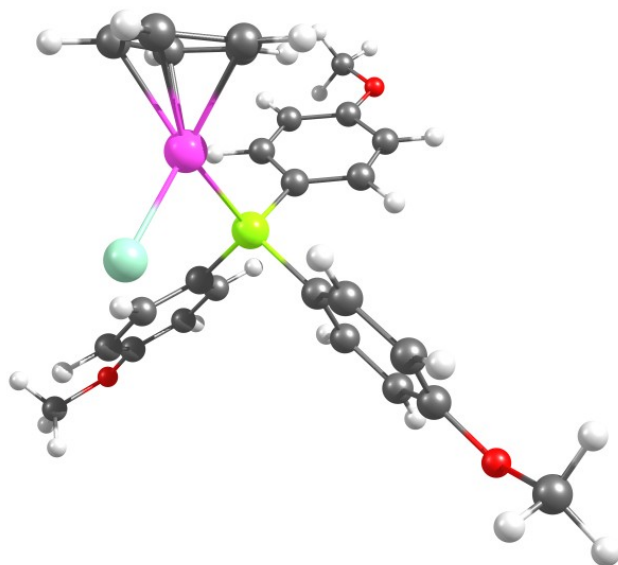
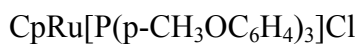
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1	-7.593018	-1.784022	-3.87406
1	-8.101123	-0.107725	-3.484009
1	-8.115477	-0.679525	-5.174402
8	-1.708237	5.961958	1.089266
6	-1.164816	6.43233	2.326501
1	-1.745008	6.061693	3.179927
1	-0.112972	6.142742	2.430868
1	-1.240641	7.519413	2.285029



Atomic Number	X	Y	Z
15	0.550224	-2.646901	0.082831
6	1.72813	-2.674679	1.52455
6	1.685927	-1.642041	2.472182
6	2.464455	-1.702474	3.633729
6	3.301877	-2.796926	3.862865
6	3.353184	-3.833389	2.923346
6	2.570102	-3.776617	1.76721
6	1.312805	-3.915488	-1.042412
6	0.65785	-5.113572	-1.375153
6	1.248429	-6.040127	-2.244312
6	2.508744	-5.78995	-2.79136
6	3.17474	-4.603344	-2.46212
6	2.580912	-3.676235	-1.602479
1	1.059945	-0.773787	2.307152
1	2.420707	-0.884161	4.347415
1	3.910888	-2.843957	4.762262
1	3.999549	-4.691489	3.091221
1	2.620468	-4.596451	1.057369
1	-0.315703	-5.351399	-0.959373
1	0.72122	-6.960008	-2.484919
1	2.968427	-6.510188	-3.463122
1	4.157598	-4.395376	-2.878219
1	3.118457	-2.76448	-1.362125
44	-0.149256	-0.649111	-1.201331
15	-2.199273	-0.124971	0.105243
15	1.577669	1.023283	-0.385248
6	0.790471	-1.318546	-3.174871
6	0.506681	0.071515	-3.284404
6	-0.902618	0.264562	-3.175882
6	-1.50049	-1.027707	-3.024194
6	-0.466519	-2.001725	-3.017105
6	-3.480928	-1.472255	0.195511
6	-3.495928	-2.551702	-0.695416
6	-4.508664	-3.519395	-0.682026
6	-5.546556	-3.422858	0.256431
6	-5.546088	-2.349116	1.166619
6	-4.536559	-1.396696	1.131639
6	-2.240864	0.453628	1.868493

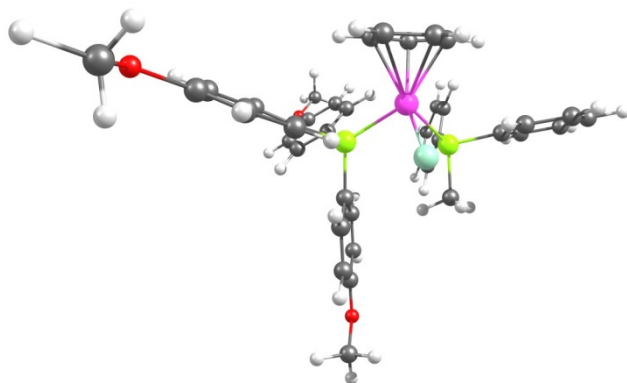
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6	-2.997425	1.952762	3.642502
6	-2.929148	1.607433	2.296058
6	-3.145851	1.203325	-0.77304
6	-2.654148	2.524897	-0.791903
6	-3.329632	3.541576	-1.454461
6	-4.525684	3.267505	-2.14563
6	-5.025858	1.958293	-2.147934
6	-4.3394	0.947799	-1.460413
6	3.24056	0.469517	-1.000688
6	3.961811	-0.538295	-0.343589
6	5.213083	-0.971187	-0.798951
6	5.766257	-0.409297	-1.959879
6	5.0465	0.58514	-2.644664
6	3.814132	1.018095	-2.166444
6	1.908111	1.535424	1.368834
6	3.175614	1.563919	1.964805
6	3.375255	2.101633	3.242764
6	2.291618	2.638145	3.952118
6	1.0147	2.629276	3.361538
6	0.835205	2.089669	2.094754
6	1.495171	2.741117	-1.102364
6	2.503432	3.676951	-0.770913
6	2.484495	4.969039	-1.271494
6	1.441695	5.389353	-2.121865
6	0.426708	4.48341	-2.453453
6	0.468898	3.178593	-1.941136
1	1.764216	-1.778091	-3.260003
1	1.240089	0.849977	-3.442541
1	-1.447999	1.192534	-3.27103
1	-2.564195	-1.214736	-2.977874
1	-0.597205	-3.074452	-2.958622
1	-2.693954	-2.663901	-1.415117
1	-4.47082	-4.335346	-1.396211
1	-6.351579	-2.28218	1.892708
1	-4.576328	-0.58208	1.847233
1	-1.126341	-1.251641	2.588209
1	-1.240628	-0.674171	4.938461
1	-3.531255	2.843738	3.961742
1	-3.436007	2.244184	1.579642
1	-1.736823	2.77531	-0.267926
1	-2.952503	4.560484	-1.444001
1	-5.946052	1.708741	-2.665088
1	-4.765284	-0.050534	-1.46413
1	3.563393	-1.000863	0.553356
1	5.737016	-1.738445	-0.238608
1	5.48058	1.020389	-3.54057
1	3.308497	1.813864	-2.70467
1	4.042229	1.180513	1.438223
1	4.376774	2.102713	3.659872
1	0.180587	3.060053	3.907639

1	-0.159594	2.115221	1.663627
1	3.317465	3.393203	-0.111154
1	3.264399	5.68024	-1.013845
1	-0.397146	4.769802	-3.098362
1	-0.33493	2.505031	-2.199158
6	-0.786926	-3.657569	0.88302
1	-1.560592	-3.948006	0.173556
1	-0.352082	-4.55066	1.340404
1	-1.271629	-3.070022	1.663179
8	2.367635	3.185	5.198202
6	3.651317	3.300085	5.816256
1	4.102133	2.315193	5.988616
1	4.328888	3.915691	5.213215
1	3.475271	3.788951	6.774943
8	1.513719	6.676498	-2.55366
6	0.482706	7.170705	-3.411808
1	0.44246	6.606391	-4.35092
1	-0.495278	7.138539	-2.917072
1	0.746533	8.207154	-3.623601
8	-5.108503	4.328945	-2.767402
6	-6.348651	4.124123	-3.450608
1	-6.234563	3.413785	-4.277929
1	-7.126272	3.771764	-2.763124
1	-6.631299	5.099384	-3.847681
8	-6.579711	-4.298427	0.371498
6	-6.639986	-5.412189	-0.522774
1	-6.720295	-5.081342	-1.564947
1	-5.765805	-6.063645	-0.405668
1	-7.539854	-5.962905	-0.247994
8	6.971173	-0.750006	-2.494507
6	7.774512	-1.715106	-1.81227
1	8.026932	-1.378182	-0.799964
1	7.273155	-2.689334	-1.763161
1	8.687495	-1.808625	-2.400915
8	-2.512798	1.569339	5.905109
6	-1.923483	0.785854	6.946259
1	-2.358159	-0.219933	6.981575
1	-0.836134	0.71791	6.823998
1	-2.151111	1.310694	7.874377



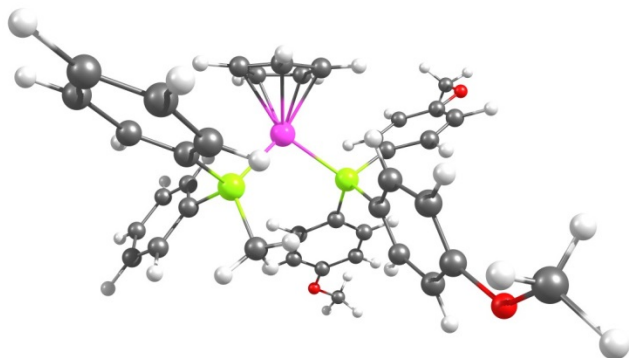
Atomic Number	X	Y	Z
44	0.464507	-0.620013	2.267584
15	-0.051811	0.024076	-0.008981
17	-1.816569	-0.621699	3.00667
6	2.554047	-0.088948	2.70172
6	2.537837	-1.287143	1.924314
6	1.804425	-2.278017	2.662511
6	1.445723	-1.714461	3.944778
6	1.88301	-0.366076	3.954586
6	1.457724	0.04478	-1.073324
6	2.432345	1.035626	-0.880582
6	3.633392	1.036607	-1.597751
6	3.887826	0.016668	-2.528315
6	2.928536	-0.989887	-2.722948
6	1.733735	-0.971682	-2.006086
6	-0.763799	1.713284	-0.246721
6	-0.480124	2.524535	-1.364087
6	-1.080073	3.77014	-1.519841
6	-1.991883	4.240862	-0.559248
6	-2.287864	3.445828	0.557028
6	-1.673049	2.197623	0.705399
6	-1.219148	-1.069814	-0.924179
6	-1.71896	-0.736303	-2.199866
6	-2.594202	-1.580389	-2.870694
6	-3.004295	-2.78929	-2.277139
6	-2.52441	-3.133467	-1.006745
6	-1.642047	-2.27065	-0.343351
1	3.022513	0.847503	2.426305
1	2.960621	-1.41313	0.936076
1	1.603336	-3.291422	2.335951
1	0.865638	-2.203607	4.717074
1	1.705973	0.352008	4.746828

1	2.257972	1.834251	-0.1631
1	4.352057	1.830081	-1.421089
1	3.135212	-1.775588	-3.444675
1	1.008125	-1.760964	-2.180495
1	0.221519	2.188653	-2.122388
1	-0.859064	4.395178	-2.380985
1	-2.987598	3.777932	1.316641
1	-1.920042	1.592884	1.574445
1	-1.428483	0.197165	-2.674086
1	-2.983449	-1.322836	-3.852004
1	-2.834706	-4.049608	-0.515748
1	-1.299874	-2.534189	0.653178
8	-2.528479	5.475348	-0.802004
6	-3.473994	5.995039	0.131173
1	-4.357432	5.349515	0.207321
1	-3.027503	6.123416	1.124828
1	-3.771423	6.969572	-0.259157
8	5.024089	-0.083543	-3.283241
6	6.029776	0.91522	-3.127509
1	5.650188	1.910747	-3.388931
1	6.425141	0.930519	-2.104234
1	6.829133	0.642032	-3.817939
8	-3.870913	-3.546723	-3.014803
6	-4.35363	-4.763875	-2.449183
1	-3.535536	-5.469321	-2.257954
1	-4.90515	-4.58117	-1.518959
1	-5.029618	-5.18922	-3.192526



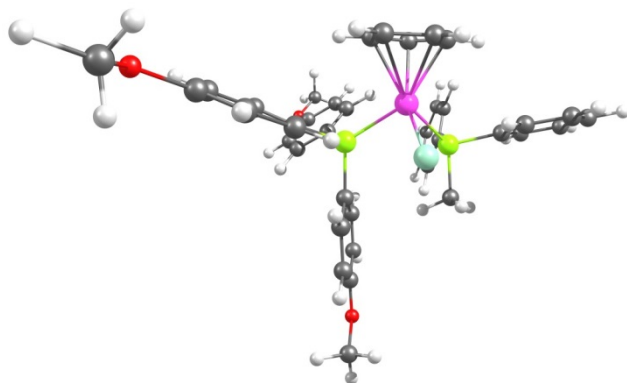
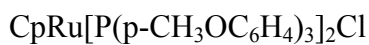
Atomic Number	X	Y	Z
44	-0.49001	-1.161779	-1.03165
15	-2.311465	-0.578621	0.380121
15	1.180918	0.181464	0.013836
17	-0.012105	-3.042762	0.569599
6	0.525346	-2.0393	-2.869318
6	0.298698	-0.647846	-3.092187
6	-1.111826	-0.404447	-3.077477
6	-1.764545	-1.67334	-2.868504
6	-0.762552	-2.66534	-2.728123
6	-3.823869	-1.628622	0.101378
6	-3.63862	-3.005555	-0.119743
6	-4.738799	-3.856419	-0.263365
6	-6.040793	-3.347072	-0.19649
6	-6.234395	-1.980987	0.029896
6	-5.134406	-1.129083	0.18478
6	-2.979972	1.140755	0.225162
6	-2.912531	2.070079	1.275226
6	-3.377895	3.380408	1.106415
6	-3.927109	3.782238	-0.113548
6	-4.00445	2.863423	-1.168581
6	-3.528189	1.561596	-1.001458
6	2.8499	-0.403282	-0.571296
6	3.15738	-1.7702	-0.466335
6	4.381912	-2.284591	-0.905911
6	5.327452	-1.432162	-1.494317
6	5.021787	-0.070726	-1.641028
6	3.804444	0.431097	-1.184548
6	1.355232	0.231049	1.862655
6	1.918404	-0.836434	2.575175
6	1.984883	-0.835023	3.973042
6	1.471933	0.250228	4.695984
6	0.892163	1.323654	4.000392
6	0.83285	1.30704	2.60972
6	1.198035	1.989187	-0.379801
6	2.162585	2.869604	0.160181
6	2.151844	4.225462	-0.139498
6	1.1634	4.754144	-0.991248

6	0.189981	3.902137	-1.526353
6	0.218999	2.536022	-1.21409
1	1.487093	-2.5323	-2.824547
1	1.067476	0.099361	-3.249459
1	-1.597539	0.53912	-3.291332
1	-2.832763	-1.841547	-2.812305
1	-0.931111	-3.711845	-2.507028
1	-2.630601	-3.41062	-0.162054
1	-4.576165	-4.919409	-0.426889
1	-6.895623	-4.008939	-0.315394
1	-7.241487	-1.57424	0.09023
1	-5.308818	-0.073169	0.370346
1	-2.50016	1.781026	2.237108
1	-3.314336	4.083099	1.934153
1	-4.296643	4.796972	-0.241274
1	-4.439778	3.160125	-2.120451
1	-3.601579	0.859958	-1.828633
1	2.420579	-2.461187	-0.063942
1	4.571101	-3.347518	-0.796149
1	5.749505	0.580729	-2.117711
1	3.603634	1.486946	-1.328885
1	2.308133	-1.700086	2.050488
1	2.430179	-1.686881	4.47581
1	0.496412	2.162414	4.567088
1	0.374883	2.152487	2.105336
1	2.926509	2.492135	0.834406
1	2.896247	4.898119	0.27812
1	-0.599521	4.278546	-2.167929
1	-0.552866	1.889008	-1.616737
6	-2.130826	-0.815938	2.203067
1	-3.067908	-0.592318	2.721951
1	-1.861869	-1.862722	2.358847
1	-1.320873	-0.204696	2.602767
8	1.236021	6.099922	-1.222155
6	0.256874	6.690965	-2.073824
1	0.296404	6.26569	-3.084251
1	-0.753964	6.570405	-1.665148
1	0.504077	7.752699	-2.119083
8	1.486336	0.358197	6.060744
6	2.055117	-0.710284	6.814282
1	1.513963	-1.650159	6.649507
1	3.115766	-0.851643	6.572003
1	1.960719	-0.418725	7.861593
8	6.55135	-1.827545	-1.964292
6	6.905564	-3.203146	-1.845397
1	6.927625	-3.522809	-0.796151
1	6.216915	-3.845472	-2.408357
1	7.907096	-3.290304	-2.269842



Atomic Number	X	Y	Z
44	0.639687	-0.100746	-1.437631
15	2.463232	0.214919	0.139017
15	-1.221267	-0.092079	0.116703
6	-0.338346	-0.597366	-3.411777
6	-0.143078	-1.777298	-2.641106
6	1.272431	-1.937525	-2.41185
6	1.956283	-0.874155	-3.10339
6	0.962514	-0.036347	-3.672242
6	3.186094	1.900432	-0.056461
6	2.858623	2.659364	-1.193646
6	3.385495	3.9423	-1.37557
6	4.250028	4.483119	-0.419438
6	4.584827	3.736626	0.716901
6	4.057032	2.455956	0.898437
6	3.8732	-0.937963	-0.153731
6	3.810888	-2.250024	0.349884
6	4.849823	-3.153552	0.107649
6	5.961947	-2.762306	-0.646403
6	6.030244	-1.460709	-1.152297
6	4.993291	-0.553006	-0.908835
6	-2.798897	-0.609008	-0.685031
6	-3.347663	0.201648	-1.6919
6	-4.524572	-0.150164	-2.357014
6	-5.178977	-1.350503	-2.026417
6	-4.639123	-2.171429	-1.0209
6	-3.470355	-1.802641	-0.360264
6	-1.632465	1.563887	0.795888
6	-2.925097	1.872947	1.252172
6	-3.234651	3.12969	1.777157
6	-2.240565	4.121535	1.847866
6	-0.944797	3.831552	1.381695
6	-0.652105	2.574664	0.866415
6	-1.057402	-1.221148	1.557981
6	-1.50616	-0.887028	2.850541
6	-1.38325	-1.783992	3.905571
6	-0.815192	-3.055428	3.699826
6	-0.359343	-3.404429	2.416604
6	-0.477986	-2.484846	1.369197

1	-1.287454	-0.203267	-3.749382
1	-0.924221	-2.435511	-2.281705
1	1.74674	-2.754901	-1.88349
1	3.027338	-0.729646	-3.153116
1	1.148993	0.884263	-4.21464
1	2.192646	2.242418	-1.947223
1	3.12121	4.516171	-2.260116
1	4.661475	5.4796	-0.557208
1	5.258717	4.151208	1.462153
1	4.338332	1.893051	1.783862
1	2.958219	-2.57444	0.942024
1	4.792582	-4.161408	0.511305
1	6.770112	-3.464601	-0.832784
1	6.894351	-1.145217	-1.731549
1	5.071525	0.458946	-1.297088
1	-2.867407	1.14129	-1.956879
1	-4.920631	0.513663	-3.118005
1	-5.158765	-3.090654	-0.765318
1	-3.09093	-2.450148	0.424557
1	-3.714925	1.129085	1.193243
1	-4.245462	3.322812	2.119772
1	-0.187068	4.60838	1.429555
1	0.357482	2.391577	0.508752
1	-1.947909	0.085938	3.042803
1	-1.725662	-1.524265	4.903373
1	0.082843	-4.375882	2.222879
1	-0.108979	-2.767484	0.385995
6	2.205469	0.063422	1.96212
1	3.151012	0.128354	2.50655
1	1.534239	0.855724	2.302384
1	1.736509	-0.895106	2.188597
8	-0.750267	-3.858069	4.792517
6	-0.206058	-5.174058	4.653011
1	-0.788392	-5.770605	3.94136
1	0.843866	-5.138159	4.339318
1	-0.271778	-5.625725	5.642863
8	-2.42757	5.374015	2.334364
6	-3.721176	5.737939	2.829493
1	-4.47753	5.683623	2.038262
1	-4.015597	5.102505	3.67243
1	-3.625529	6.769238	3.169137
8	-6.32336	-1.796501	-2.607006
6	-6.935919	-1.001408	-3.626698
1	-7.231641	-0.019257	-3.240018
1	-6.269332	-0.877545	-4.488236
1	-7.825189	-1.551878	-3.934086



Atomic Number	X	Y	Z
44	-0.199945	-0.762987	-1.593956
15	1.778204	-0.235068	-0.343269
15	-1.93287	0.114981	-0.18879
6	-1.351436	-1.917471	-3.182751
6	-1.38541	-2.655417	-1.958898
6	-0.048853	-3.021796	-1.60491
6	0.820394	-2.52224	-2.641959
6	0.021922	-1.839012	-3.595002
6	3.286674	0.041084	-1.395114
6	3.197946	0.11654	-2.79577
6	4.326812	0.350156	-3.578258
6	5.582906	0.520572	-2.977109
6	5.690398	0.465568	-1.578125
6	4.546548	0.236446	-0.808306
6	1.970026	1.223743	0.784915
6	1.661374	2.492587	0.249918
6	1.893605	3.651016	0.98022
6	2.429338	3.578098	2.276715
6	2.738657	2.32853	2.82631
6	2.51291	1.16619	2.073663
6	2.28005	-1.678603	0.704471
6	1.571338	-1.966896	1.889091
6	1.853076	-3.096528	2.649067
6	2.848482	-3.999318	2.23463
6	3.553072	-3.742942	1.052241
6	3.265999	-2.589995	0.306796
6	-3.518157	0.128333	-1.170948
6	-3.520724	0.723964	-2.451856
6	-4.672458	0.759628	-3.229552
6	-5.864524	0.178062	-2.764392
6	-5.876115	-0.44443	-1.510688
6	-4.710313	-0.460237	-0.730391
6	-1.867636	1.829232	0.514401
6	-2.259714	2.954415	-0.235581
6	-2.178525	4.238113	0.293907
6	-1.692625	4.440072	1.595575
6	-1.287952	3.334661	2.354969

6	-1.369146	2.050931	1.805584
6	-2.415096	-0.861064	1.315196
6	-3.363762	-0.385593	2.248443
6	-3.742047	-1.1449	3.348493
6	-3.182305	-2.419532	3.556264
6	-2.23714	-2.909772	2.647064
6	-1.866961	-2.12647	1.544253
1	-2.202988	-1.503097	-3.705572
1	-2.280655	-2.903899	-1.401709
1	0.255543	-3.626384	-0.759751
1	1.894689	-2.648273	-2.687007
1	0.383564	-1.310725	-4.46854
1	2.229354	0.033712	-3.275066
1	4.25119	0.421412	-4.659977
1	6.643256	0.608468	-1.079237
1	4.652196	0.215502	0.273469
1	1.237001	2.569258	-0.748104
1	1.654479	4.626111	0.564929
1	3.158344	2.236731	3.822909
1	2.786024	0.212897	2.515406
1	0.783503	-1.299391	2.225502
1	1.310076	-3.301132	3.568073
1	4.324302	-4.418527	0.69732
1	3.834075	-2.41269	-0.601331
1	-2.602687	1.148763	-2.850497
1	-4.666107	1.227729	-4.210536
1	-6.771929	-0.9193	-1.124195
1	-4.75658	-0.956441	0.232848
1	-2.630412	2.837983	-1.246853
1	-2.481443	5.102023	-0.291548
1	-0.893776	3.452318	3.358398
1	-1.036004	1.215824	2.414408
1	-3.809423	0.595891	2.1151
1	-4.471445	-0.772081	4.062715
1	-1.776348	-3.883098	2.779263
1	-1.118462	-2.511074	0.860411
17	-0.06995	1.466053	-2.747671
8	6.631674	0.743402	-3.828832
6	7.921526	0.969768	-3.267801
1	7.927836	1.854965	-2.619651
1	8.272442	0.098585	-2.7001
1	8.588819	1.138936	-4.114561
8	3.046685	-5.085907	3.045315
6	4.0449	-6.031547	2.668694
1	3.816323	-6.492016	1.699417
1	5.039474	-5.570176	2.628642
1	4.035197	-6.799707	3.443612
8	2.599004	4.777535	2.925365
6	3.237043	4.766595	4.1987
1	2.649355	4.212307	4.941953
1	4.244309	4.335539	4.138447
1	3.3106	5.811391	4.505868
8	-3.619015	-3.088241	4.666468

6	-3.086205	-4.385369	4.925294
1	-3.316281	-5.083192	4.11079
1	-2.000785	-4.349153	5.080343
1	-3.569717	-4.728111	5.841356
8	-6.941294	0.261869	-3.606492
6	-8.173712	-0.312546	-3.181823
1	-8.080242	-1.39488	-3.02654
1	-8.540321	0.158138	-2.260877
1	-8.883838	-0.125163	-3.988996
8	-1.646574	5.740232	2.023523
6	-1.065296	6.008624	3.297592
1	-1.637241	5.537029	4.107262
1	-0.021208	5.675341	3.337191
1	-1.10446	7.092869	3.418234

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