Electronic Supplementary Information for Dalton Transactions

DFT calculations of 1H and 13C NMR chemical shifts in transition metal hydrides

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Trans-Ru(H_2)($dppm)_2$

C	-2.743443	1.555201	0.770608
P	-2.583488	3.287340	0.107168
C	-0.811181	3.339098	-0.436465
Ru	-4.304275	4.401281	-0.972832
P	-3.998438	5.479149	1.054284
C	-5.214743	5.427213	2.453841
P	-4.637764	3.299449	-2.982237
C	-3.400758	3.328557	-4.373025
P	-5.994351	5.542490	-2.071309
C	-7.759460	5.570143	-1.479501
C	-6.033778	4.419195	-3.588312
C	-5.363902	1.599581	-3.139368
C	-2.595757	4.366422	1.656902
C	-5.801565	7.235871	-2.803855
C	-3.301669	7.199301	1.200405
H	-5.436765	3.395423	-0.260610
H	-3.170332	5.404062	-1.684535
H	-6.976010	3.879387	-3.702550
H	-5.802536	4.949345	-4.514385
H	-1.653534	4.896333	1.811245
H	-2.859564	3.816852	2.562744
C	-4.836571	5.710990	3.779371
C	-5.770053	5.623383	4.815075
C	-7.093179	5.257722	4.537048
C	-7.475900	4.974438	3.223546
C	-6.539085	5.053273	2.185668
H	-3.817353	6.004078	4.001436
H	-5.468355	5.839387	5.832505
H	-7.816391	5.192184	5.340390
H	-8.496254	4.689355	3.001376
H	-6.819007	4.806658	1.169428
C	-3.983888	8.246110	1.841466
C	-3.442365	9.536928	1.867187
C	-2.211787	9.796789	1.259208
C	-1.529465	8.762043	0.608432
C	-2.075150	7.476741	0.569230
H	-4.935034	8.058433	2.321527
H	-3.982580	10.333340	2.363800
H	-1.790550	10.793894	1.286251
H	-0.579351	8.955502	0.126112
H	-1.562607	6.692912	0.024522
C	-6.669612	7.714807	-3.802656
C	-6.474561	8.979920	-4.362042
C	-5.413851	9.783306	-3.924839
C	-4.548081	9.314665	-2.933414
C	-4.737302	8.043021	-2.377952
H	-7.498263	7.103073	-4.139123
H	-7.145383	9.337715	-5.133282
H	-5.264829	10.764821	-4.357380
H	-3.725330	9.929750	-2.591988
H	-4.054386	7.659031	-1.630706
C	-8.447412	6.759962	-1.190585
C	-9.750559	6.721453	-0.680340
C	-10.384405	5.496564	-0.457944
C	-9.703372	4.305065	-0.734129
C	-8.398114	4.341345	-1.230366
H	-7.970872	7.716079	-1.361472
H	-10.265798	7.648078	-0.459865

H	-11.394769	5.468652	-0.069657
H	-10.182796	3.350297	-0.557047
H	-7.862615	3.414390	-1.397320
C	-2.834943	2.162246	-4.913309
C	-1.855326	2.243274	-5.910380
C	-1.432520	3.488041	-6.383041
C	-1.982999	4.656429	-5.843059
C	-2.951002	4.577679	-4.839036
H	-3.155255	1.191239	-4.559978
H	-1.427743	1.334199	-6.314670
H	-0.679901	3.549135	-7.159083
H	-1.655304	5.626303	-6.196171
H	-3.338260	5.487564	-4.396444
C	-5.918251	1.141656	-4.349235
C	-6.496107	-0.127728	-4.426361
C	-6.520417	-0.956117	-3.297174
C	-5.972113	-0.508172	-2.092738
C	-5.399917	0.767523	-2.011853
H	-5.893876	1.773592	-5.229016
H	-6.923734	-0.469804	-5.360669
H	-6.966074	-1.941161	-3.358581
H	-5.988910	-1.142701	-1.215887
H	-4.998416	1.134683	-1.076274
C	-0.517406	3.710762	-1.755897
C	0.811912	3.789868	-2.189081
C	1.855924	3.508931	-1.304001
C	1.571560	3.143500	0.017775
C	0.245455	3.055388	0.448590
H	-1.331961	3.955313	-2.425314
H	1.024569	4.074261	-3.211638
H	2.884099	3.575629	-1.637322
H	2.378151	2.928179	0.707612
H	0.032456	2.762107	1.469679
C	-3.836966	1.267210	1.607995
C	-4.033749	-0.023941	2.103184
C	-3.153454	-1.054126	1.751426
C	-2.078619	-0.783286	0.901178
C	-1.871699	0.513371	0.415071
H	-4.548431	2.048589	1.847983
H	-4.875237	-0.225496	2.754378
H	-3.307971	-2.056010	2.131852
H	-1.398461	-1.575948	0.615108
H	-1.032736	0.708757	-0.239427

Cis-Ru(H_2)(dppm)$_2$

C	-0.474609	0.726611	-0.314083
P	-0.685219	0.380954	1.511254
C	1.077360	0.584491	2.084320
Ru	-2.409197	-1.050637	2.290001
P	-2.718660	1.008592	3.296225
C	-4.308787	1.959275	3.199871
P	-2.011736	-2.663085	3.984702
C	-0.435121	-3.134926	4.861958
P	-2.174230	-3.098881	1.244847
C	-0.606475	-3.670620	0.431949
C	-2.314311	-4.121710	2.816410
C	-3.244736	-2.936164	5.362711
C	-1.536221	1.938664	2.169660
C	-3.452968	-3.808799	0.103089

C	-2.162666	1.408229	5.021195
H	-3.935819	-1.509460	2.557962
H	-3.178576	-0.402449	1.025004
H	-0.904944	2.703261	2.627188
H	-2.120523	2.393172	1.366816
H	-1.655627	-4.987602	2.910213
H	-3.350983	-4.450410	2.916289
C	-3.068319	1.235235	6.083982
C	-2.665227	1.447662	7.404544
C	-1.350298	1.832981	7.686215
C	-0.439907	1.998048	6.638929
C	-0.841169	1.783908	5.315500
H	-4.088292	0.935919	5.878687
H	-3.375960	1.309745	8.209508
H	-1.039130	1.999557	8.709717
H	0.581176	2.293187	6.846733
H	-0.114875	1.903414	4.522013
C	-4.417348	3.279800	3.671705
C	-5.617242	3.981651	3.533217
C	-6.722587	3.369965	2.929141
C	-6.623293	2.056317	2.463170
C	-5.419862	1.353380	2.595587
H	-3.571275	3.753944	4.153783
H	-5.691589	4.998834	3.897317
H	-7.652849	3.914568	2.825936
H	-7.477010	1.578442	1.999019
H	-5.322280	0.337024	2.234229
C	-2.866759	-3.107811	6.704531
C	-3.834851	-3.275828	7.701781
C	-5.192322	-3.283557	7.373074
C	-5.579812	-3.107465	6.040018
C	-4.615415	-2.924568	5.046258
H	-1.820636	-3.107933	6.977616
H	-3.523639	-3.402490	8.731366
H	-5.939826	-3.418907	8.144702
H	-6.629807	-3.101853	5.774777
H	-4.921633	-2.744178	4.023154
C	0.456125	-2.114369	5.227340
C	1.639035	-2.412296	5.913991
C	1.951534	-3.737018	6.231511
C	1.071333	-4.764026	5.871004
C	-0.116959	-4.463811	5.198456
H	0.223609	-1.089214	4.969321
H	2.312856	-1.611761	6.191512
H	2.869286	-3.968956	6.757301
H	1.304377	-5.791902	6.120271
H	-0.803017	-5.265502	4.954008
C	-3.363713	-5.122866	-0.390056
C	-4.371222	-5.639093	-1.208551
C	-5.474622	-4.846643	-1.548170
C	-5.567221	-3.538439	-1.065810
C	-4.561170	-3.021147	-0.240966
H	-2.505638	-5.736168	-0.144116
H	-4.295312	-6.652634	-1.582321
H	-6.253079	-5.247399	-2.185370
H	-6.416907	-2.920945	-1.329231
H	-4.618687	-2.011339	0.146451
C	0.454314	-4.229710	1.164084
C	1.652036	-4.577534	0.529672
C	1.809732	-4.363775	-0.842385

C	0.764660	-3.794668	-1.577663
C	-0.432954	-3.449478	-0.946634
H	0.360198	-4.389173	2.230391
H	2.456420	-5.014178	1.108603
H	2.736296	-4.634085	-1.332823
H	0.880163	-3.617658	-2.639484
H	-1.234283	-3.009254	-1.526258
C	-1.627975	0.910630	-1.098420
C	-1.527378	1.160918	-2.469051
C	-0.271978	1.210337	-3.085261
C	0.878748	1.007217	-2.320112
C	0.780032	0.770644	-0.943848
H	-2.603150	0.829572	-0.633810
H	-2.426907	1.307229	-3.054130
H	-0.193778	1.399036	-4.148653
H	1.855027	1.034138	-2.788199
H	1.681920	0.618964	-0.367282
C	1.718595	1.835322	2.148793
C	3.048072	1.933989	2.569805
C	3.760550	0.780534	2.918085
C	3.137190	-0.468208	2.845672
C	1.801602	-0.564361	2.437199
H	1.189607	2.732531	1.851850
H	3.527556	2.903948	2.617050
H	4.791824	0.856450	3.239375
H	3.681712	-1.365484	3.110835
H	1.316557	-1.531006	2.394303

Trans-Ru(HCl)(dppm)$_2$

C	-1.626582	0.484644	0.266566
C	-2.628913	1.344424	0.749121
C	-3.635293	0.818792	1.581508
C	-3.615030	-0.530359	1.946719
C	-2.604508	-1.375289	1.476028
C	-1.615756	-0.866130	0.629501
P	-2.732747	3.124410	0.230537
C	-2.881779	4.096419	1.839163
P	-4.148940	5.333084	1.188748
C	-3.254051	6.959374	1.175630
C	-3.865047	8.136119	1.640852
C	-3.198659	9.363746	1.556688
C	-1.913011	9.431821	1.013337
C	-1.298472	8.265888	0.543186
C	-1.966214	7.040361	0.615846
C	-0.996206	3.468126	-0.317559
C	-0.752119	3.892533	-1.631634
C	0.554964	4.158826	-2.058319
C	1.625661	4.012206	-1.172913
C	1.390811	3.592480	0.142417
C	0.088633	3.317637	0.566406
Ru	-4.551381	4.178959	-0.807660
P	-6.174114	5.409437	-1.966238
C	-5.746237	6.996581	-2.822789
C	-6.519602	7.462346	-3.902688
C	-6.184233	8.651393	-4.553924
C	-5.075606	9.394018	-4.128718
C	-4.305439	8.941457	-3.054481
C	-4.636168	7.745212	-2.405257

P	-4.819183	3.150965	-2.896380
C	-5.335285	1.406211	-3.225325
C	-5.830853	1.022404	-4.485317
C	-6.231623	-0.295529	-4.713096
C	-6.137847	-1.242803	-3.685335
C	-5.649079	-0.866477	-2.432283
C	-5.251830	0.455932	-2.198015
C	-5.327792	5.557248	2.595271
C	-4.864232	5.857793	3.889530
C	-5.766519	6.008520	4.944431
C	-7.140720	5.862879	4.715527
C	-7.606173	5.561782	3.433563
C	-6.703787	5.403874	2.374330
C	-3.586517	3.442258	-4.253079
C	-2.786664	2.395063	-4.742216
C	-1.806721	2.641622	-5.709823
C	-1.615201	3.934663	-6.204727
C	-2.403397	4.984118	-5.720081
C	-3.376989	4.742028	-4.746812
C	-6.322920	4.177668	-3.386221
C	-7.920977	5.729108	-1.421908
C	-8.413825	7.032295	-1.232443
C	-9.716703	7.237258	-0.766708
C	-10.542005	6.145688	-0.481803
C	-10.052886	4.846004	-0.648883
C	-8.749407	4.635186	-1.107788
Cl	-6.276143	2.656269	0.291839
H	-3.473167	5.129677	-1.492379
H	-7.215005	3.562666	-3.249144
H	-6.319169	4.601686	-4.392679
H	-1.952117	4.514444	2.230861
H	-3.358691	3.479032	2.603531
H	-3.803349	5.982355	4.070964
H	-5.401663	6.238745	5.937675
H	-7.840292	5.979229	5.533873
H	-8.665812	5.437057	3.252443
H	-7.059396	5.127755	1.391611
H	-4.855840	8.095070	2.073699
H	-3.684090	10.261000	1.919688
H	-1.395424	10.381119	0.956410
H	-0.303672	8.307470	0.117679
H	-1.486885	6.152661	0.223181
H	-7.388563	6.902486	-4.226677
H	-6.784625	8.998283	-5.385577
H	-4.817088	10.317104	-4.632255
H	-3.448262	9.510670	-2.718663
H	-4.028601	7.381846	-1.587156
H	-7.787255	7.886656	-1.451010
H	-10.082998	8.247141	-0.630312
H	-11.552366	6.305595	-0.126790
H	-10.677391	3.993805	-0.412502
H	-8.363631	3.626456	-1.174698
H	-2.931924	1.387634	-4.374743
H	-1.199922	1.823171	-6.076396
H	-0.861791	4.123106	-6.959161
H	-2.261495	5.990130	-6.094498
H	-3.960769	5.570020	-4.365730
H	-5.893199	1.747855	-5.287672
H	-6.612529	-0.583162	-5.685140
H	-6.448421	-2.264936	-3.862587

H	-5.583624	-1.591264	-1.631240
H	-4.913852	0.759994	-1.217253
H	-1.586329	4.027953	-2.306802
H	0.728244	4.481843	-3.076707
H	2.635719	4.222823	-1.501368
H	2.217445	3.477399	0.832266
H	-0.081856	2.977767	1.580791
H	-4.456577	1.446943	1.901122
H	-4.396201	-0.919112	2.587673
H	-2.592144	-2.420012	1.760352
H	-0.835024	-1.514782	0.252176
H	-0.853233	0.864868	-0.387330

Cis-Ru(HCl)(dppm)$_2$

C	1.751799	-0.746453	1.406595
C	0.990162	0.243409	2.057060
C	1.634346	1.084673	2.978854
C	3.002953	0.943427	3.243342
C	3.747659	-0.039148	2.586889
C	3.116207	-0.884367	1.667305
P	-0.826738	0.341125	1.636407
C	-1.445762	1.929731	2.440534
P	-2.879284	1.105034	3.340654
C	-2.580872	1.458404	5.137909
C	-3.626516	1.847191	5.991454
C	-3.392379	2.042992	7.356716
C	-2.113409	1.856980	7.887473
C	-1.067965	1.457217	7.048045
C	-1.302847	1.250081	5.686363
C	-0.665472	0.809652	-0.164521
C	-1.593786	0.337835	-1.104048
C	-1.507647	0.725493	-2.446431
C	-0.495441	1.593383	-2.863095
C	0.434337	2.071963	-1.932833
C	0.353104	1.680062	-0.594315
Ru	-2.559738	-0.977464	2.340654
P	-2.213119	-3.055496	1.296792
C	-3.393417	-3.786874	0.071266
C	-3.226157	-5.096395	-0.413234
C	-4.140382	-5.632880	-1.322827
C	-5.225841	-4.864414	-1.760511
C	-5.396160	-3.562408	-1.282783
C	-4.485395	-3.023602	-0.366616
P	-2.007008	-2.656381	4.069272
C	-3.019980	-2.960935	5.596766
C	-2.575433	-2.380934	6.799145
C	-3.311384	-2.528738	7.976442
C	-4.503850	-3.259702	7.971464
C	-4.956856	-3.832751	6.780945
C	-4.224513	-3.680664	5.598339
C	-4.319752	2.198965	2.954446
C	-4.253694	3.585997	3.183137
C	-5.327879	4.409254	2.838754
C	-6.480371	3.853900	2.268864
C	-6.552823	2.476940	2.044913
C	-5.475650	1.647509	2.382348
C	-0.345008	-3.182075	4.725455
C	0.763494	-2.335504	4.600394
C	2.014412	-2.721374	5.100401

C	2.166283	-3.960879	5.725065
C	1.063861	-4.815880	5.854502
C	-0.183722	-4.427318	5.362816
C	-2.414381	-4.056269	2.871342
C	-0.591367	-3.592939	0.573788
C	0.396668	-4.253404	1.321450
C	1.618081	-4.604123	0.733757
C	1.871395	-4.294847	-0.604938
C	0.896878	-3.627823	-1.356793
C	-0.323402	-3.279861	-0.773016
Cl	-4.850667	-1.777931	2.846054
H	-3.258597	-0.312246	1.071416
H	-0.746572	2.464248	3.084423
H	-1.820151	2.614296	1.676928
H	-1.843607	-4.980850	2.974142
H	-3.483510	-4.264475	2.935986
H	-4.621272	1.995851	5.593420
H	-4.210360	2.339830	8.000879
H	-1.933342	2.015611	8.943172
H	-0.075172	1.300630	7.451439
H	-0.490086	0.907913	5.057481
H	-3.369022	4.021020	3.632909
H	-5.267620	5.476168	3.014060
H	-7.313584	4.492559	2.003284
H	-7.443307	2.042639	1.608389
H	-5.525682	0.578189	2.216784
H	-1.652967	-1.814712	6.817815
H	-2.954841	-2.072568	8.891269
H	-5.075200	-3.376306	8.883795
H	-5.884991	-4.390044	6.763856
H	-4.614245	-4.100189	4.682915
H	0.650919	-1.383647	4.100679
H	2.860158	-2.054931	4.992880
H	3.132349	-4.260656	6.111657
H	1.174910	-5.775369	6.344213
H	-1.037348	-5.081702	5.491087
H	-2.379493	-5.689930	-0.090855
H	-4.005404	-6.642475	-1.690338
H	-5.933113	-5.280413	-2.467122
H	-6.238640	-2.967744	-1.612367
H	-4.627513	-2.029582	0.036149
H	0.232194	-4.487706	2.363886
H	2.365202	-5.117435	1.325721
H	2.814091	-4.571734	-1.059769
H	1.083372	-3.381518	-2.394355
H	-1.070900	-2.770579	-1.367511
H	-2.387653	-0.318229	-0.771753
H	-2.232549	0.352073	-3.158896
H	-0.429832	1.895521	-3.900793
H	1.221707	2.745090	-2.248432
H	1.087542	2.044213	0.112839
H	1.087859	1.863646	3.492939
H	3.481755	1.607379	3.952368
H	4.807020	-0.142801	2.784940
H	3.681606	-1.650180	1.152552
H	1.279259	-1.405367	0.689810

Trans-[Ru(H-H_2O)(dppm)$_2$]$^+$

C	-8.452037	4.105821	-1.757346
C	-7.823349	5.361826	-1.645356

C	-8.541082	6.428986	-1.074864
C	-9.858113	6.246551	-0.639936
C	-10.475583	4.997882	-0.761792
C	-9.769968	3.928049	-1.321896
P	-6.038917	5.554481	-2.114106
C	-5.861958	4.568785	-3.708939
P	-4.618024	3.333849	-3.022622
C	-3.300929	3.244367	-4.318642
C	-2.899565	2.029597	-4.895898
C	-1.891241	2.010564	-5.866216
C	-1.280618	3.199856	-6.271444
C	-1.672642	4.414233	-5.696281
C	-2.671105	4.437077	-4.719634
Ru	-4.391920	4.369384	-0.930601
O	-5.915441	2.976159	0.132213
P	-2.586455	3.303735	0.157015
C	-0.834660	3.443994	-0.395799
C	-0.538958	3.852753	-1.703534
C	0.792829	3.975610	-2.118436
C	1.832624	3.696481	-1.228734
C	1.543868	3.288109	0.079687
C	0.217563	3.159041	0.495119
C	-2.696983	1.553716	0.760430
C	-1.891912	0.545028	0.201235
C	-2.033828	-0.784177	0.613573
C	-2.978689	-1.123421	1.586491
C	-3.791267	-0.128368	2.140621
C	-3.658057	1.200472	1.726633
C	-2.661796	4.365393	1.710082
P	-3.981992	5.551585	1.076164
C	-5.211220	5.662106	2.450213
C	-4.817613	5.652438	3.800341
C	-5.774899	5.735046	4.815006
C	-7.133585	5.833778	4.493698
C	-7.533102	5.853538	3.154742
C	-6.576005	5.765583	2.137704
C	-3.155927	7.206281	1.101311
C	-3.696210	8.300220	1.795785
C	-3.046849	9.539856	1.772556
C	-1.853982	9.697353	1.062567
C	-1.312295	8.611908	0.364211
C	-1.961849	7.375324	0.376156
C	-5.912146	7.313370	-2.640055
C	-6.818134	7.856503	-3.570961
C	-6.674348	9.176992	-4.000045
C	-5.629100	9.966599	-3.503906
C	-4.727303	9.432391	-2.580753
C	-4.865085	8.107239	-2.150079
C	-5.445559	1.682766	-3.137985
C	-6.345272	1.351096	-4.166234
C	-6.946484	0.089237	-4.199918
C	-6.652795	-0.857738	-3.212332
C	-5.748028	-0.544446	-2.193656
C	-5.148219	0.720412	-2.154811
H	-3.335324	5.317383	-1.617392
H	-6.790294	4.141336	-4.091321
H	-5.412868	5.188178	-4.487891
H	-1.711691	4.842368	1.957452
H	-3.017177	3.798649	2.572542
H	-3.768905	5.591622	4.063731

H	-5.461872	5.726917	5.850993
H	-7.872363	5.897951	5.281781
H	-8.581714	5.936574	2.900170
H	-6.890724	5.789709	1.101558
H	-4.614259	8.190016	2.356971
H	-3.471634	10.375412	2.313634
H	-1.349444	10.654711	1.053862
H	-0.388194	8.726355	-0.187617
H	-1.542490	6.549129	-0.185257
H	-7.633881	7.255904	-3.954301
H	-7.372966	9.588973	-4.716656
H	-5.521356	10.990513	-3.837424
H	-3.918918	10.038417	-2.193747
H	-4.161076	7.689189	-1.443198
H	-8.080987	7.404870	-0.987262
H	-10.401821	7.082041	-0.218108
H	-11.497163	4.861589	-0.432408
H	-10.245248	2.961512	-1.430662
H	-7.928912	3.266833	-2.202020
H	-3.372744	1.102556	-4.600959
H	-1.591480	1.068593	-6.306747
H	-0.507879	3.182663	-7.028768
H	-1.204627	5.339532	-6.006886
H	-2.951415	5.380895	-4.266575
H	-6.566255	2.063334	-4.951105
H	-7.635256	-0.156008	-4.997924
H	-7.118874	-1.833789	-3.242998
H	-5.502010	-1.278053	-1.437052
H	-4.421512	0.947088	-1.381890
H	-1.344749	4.074348	-2.389347
H	1.010793	4.285927	-3.131832
H	2.861850	3.793481	-1.548966
H	2.347928	3.069147	0.770215
H	0.003423	2.828696	1.504322
H	-4.309734	1.953329	2.150913
H	-4.523326	-0.383195	2.896302
H	-3.077855	-2.150250	1.913472
H	-1.399441	-1.547874	0.182521
H	-1.146274	0.795231	-0.541978
H	-6.788484	3.347155	0.303599
H	-6.012133	2.097050	-0.253648

Cis-[Ru(H-H_2O)(dppm)$_2$]$^+$

C	1.596395	-0.775727	2.952250
C	1.098939	0.309122	2.220889
C	1.934588	1.419699	1.990980
C	3.240963	1.433225	2.484209
C	3.729909	0.339393	3.209857
C	2.907164	-0.764478	3.444270
P	-0.636367	0.295416	1.579522
C	-1.330764	1.925481	2.203884
P	-2.591396	1.149083	3.355643
C	-2.019245	1.550536	5.069495
C	-2.952669	1.497404	6.121752
C	-2.554579	1.752008	7.436520
C	-1.220270	2.064060	7.719906
C	-0.285428	2.113710	6.682343
C	-0.679364	1.853462	5.364426
C	-0.397208	0.530485	-0.245085

C	-1.476978	0.985724	-1.022630
C	-1.328054	1.185011	-2.396528
C	-0.103602	0.913900	-3.016755
C	0.967919	0.442331	-2.255760
C	0.825875	0.253921	-0.876470
Ru	-2.380463	-0.974311	2.327678
P	-1.960766	-2.966784	1.164504
C	-3.450013	-3.821078	0.467503
C	-3.588621	-5.219632	0.446767
C	-4.732525	-5.807738	-0.101192
C	-5.746055	-5.008565	-0.642739
C	-5.610752	-3.617290	-0.643974
C	-4.469186	-3.024588	-0.089215
P	-1.753569	-2.702986	3.967300
C	-3.196254	-3.388875	4.928486
C	-3.428024	-2.892782	6.226680
C	-4.521753	-3.336317	6.973788
C	-5.410060	-4.275077	6.437010
C	-5.200622	-4.764606	5.145778
C	-4.103703	-4.323294	4.393068
C	-4.102631	2.194251	3.192930
C	-4.096188	3.543548	3.591533
C	-5.232789	4.333514	3.408696
C	-6.386116	3.783082	2.836078
C	-6.400286	2.441802	2.445760
C	-5.261200	1.647009	2.620632
C	-0.406192	-2.929497	5.213932
C	0.064619	-1.812596	5.921698
C	1.041443	-1.967734	6.911925
C	1.560897	-3.234167	7.192181
C	1.098994	-4.351402	6.485862
C	0.115490	-4.202496	5.505327
C	-1.418135	-3.999252	2.642748
C	-0.684779	-3.287181	-0.137809
C	0.679881	-3.327811	0.196346
C	1.643842	-3.563764	-0.787210
C	1.258668	-3.745093	-2.118764
C	-0.094264	-3.685599	-2.462592
C	-1.062394	-3.460902	-1.479710
O	-4.497852	-1.607268	2.747643
H	-3.027639	-0.242565	1.055282
H	-0.614483	2.620116	2.644842
H	-1.873109	2.429154	1.401692
H	-0.343705	-4.187886	2.590116
H	-1.922468	-4.959149	2.768925
H	-3.992794	1.280111	5.912171
H	-3.285590	1.719727	8.234107
H	-0.915687	2.273516	8.736937
H	0.747106	2.362493	6.891677
H	0.065630	1.888888	4.580274
H	-3.212886	3.972966	4.047830
H	-5.220878	5.371931	3.713471
H	-7.266611	4.397300	2.699143
H	-7.293328	2.013953	2.008565
H	-5.262543	0.606602	2.326225
H	-2.744585	-2.174249	6.660999
H	-4.675493	-2.954832	7.974755
H	-6.253070	-4.621585	7.019847
H	-5.880468	-5.492820	4.722609
H	-3.963025	-4.722241	3.396337

H	-0.324679	-0.827391	5.699247
H	1.393743	-1.101391	7.456059
H	2.317770	-3.353396	7.956464
H	1.496099	-5.334138	6.704716
H	-0.251491	-5.077785	4.983860
H	-2.800778	-5.853653	0.833893
H	-4.828318	-6.885694	-0.114259
H	-6.628020	-5.468270	-1.068720
H	-6.382819	-2.996084	-1.079464
H	-4.343315	-1.946477	-0.117030
H	1.006141	-3.171552	1.216578
H	2.689913	-3.605280	-0.512466
H	2.005189	-3.931343	-2.879583
H	-0.400184	-3.821595	-3.491611
H	-2.106428	-3.432790	-1.760840
H	-2.438598	1.171598	-0.560571
H	-2.164515	1.548383	-2.979555
H	0.011447	1.067556	-4.081800
H	1.916158	0.223235	-2.728944
H	1.668037	-0.105596	-0.302049
H	1.574942	2.264313	1.415881
H	3.875952	2.290190	2.300278
H	4.743467	0.351909	3.589012
H	3.274806	-1.607846	4.013800
H	0.949937	-1.617393	3.158323
H	-4.678114	-2.051651	3.588154
H	-4.895784	-2.119002	2.030314

Trans-Ru(H_2)(dppm)($PPh3)_2$

C	-3.766273	1.400451	0.989320
C	-3.342024	2.624032	0.445928
C	-2.060527	2.696840	-0.131244
C	-1.240053	1.567576	-0.194347
C	-1.681096	0.348404	0.331684
C	-2.941475	0.271518	0.929242
P	-4.356979	4.182435	0.552701
C	-4.129539	4.962252	-1.135836
P	-3.567257	6.618635	-0.462593
C	-4.652902	7.831756	-1.369353
C	-4.168890	9.024608	-1.928827
C	-5.039319	9.914828	-2.567880
C	-6.404578	9.631310	-2.650369
C	-6.901396	8.456676	-2.074785
C	-6.033907	7.568478	-1.434038
C	-6.110496	3.565883	0.345139
C	-7.166552	4.327278	0.868066
C	-8.496573	3.972897	0.614080
C	-8.787805	2.853861	-0.171105
C	-7.742036	2.097517	-0.710948
C	-6.413164	2.452222	-0.459802
Ru	-3.759578	6.066254	1.795687
P	-3.495545	8.324745	2.519865
C	-5.063547	9.184543	3.080861
C	-5.201008	9.873052	4.296524
C	-6.411138	10.493095	4.634478
C	-7.498339	10.443251	3.759541
C	-7.374956	9.753583	2.548101
C	-6.173574	9.121848	2.217421
P	-3.682996	4.865985	3.858593

C	-1.964336	4.421687	4.457500
C	-1.470258	4.693107	5.742717
C	-0.167959	4.319864	6.101279
C	0.655313	3.661986	5.185002
C	0.175611	3.393667	3.898069
C	-1.116935	3.779488	3.535051
C	-1.932819	6.756461	-1.362587
C	-1.874036	6.971312	-2.752382
C	-0.648731	6.941007	-3.424613
C	0.534441	6.686625	-2.722008
C	0.483487	6.453200	-1.345122
C	-0.743101	6.484953	-0.671132
C	-4.473764	3.160695	3.922058
C	-3.797209	1.991679	4.304391
C	-4.487532	0.781068	4.442184
C	-5.861271	0.718972	4.196724
C	-6.545948	1.879209	3.817456
C	-5.858124	3.087930	3.688120
C	-2.886201	9.593265	1.272933
C	-3.586636	10.758831	0.926540
C	-3.006579	11.715071	0.083636
C	-1.721902	11.519847	-0.428459
C	-1.014798	10.360246	-0.090118
C	-1.591226	9.410751	0.756506
H	-2.115283	5.818541	1.833380
H	-5.380304	6.393095	1.982996
H	-5.068043	5.009908	-1.689248
H	-3.373280	4.480749	-1.756799
H	-2.781074	7.158930	-3.312259
H	-0.619910	7.111493	-4.493717
H	1.482535	6.664404	-3.244728
H	1.392189	6.245157	-0.793757
H	-0.800846	6.282537	0.393133
H	-3.116797	9.266573	-1.862429
H	-4.646012	10.829580	-2.992862
H	-7.075441	10.319179	-3.149454
H	-7.959471	8.231050	-2.123227
H	-6.437828	6.675705	-0.971918
H	-4.378662	9.911786	4.996603
H	-6.496913	11.012667	5.580987
H	-8.431277	10.927615	4.019464
H	-8.212106	9.700457	1.863369
H	-6.097048	8.561732	1.295038
H	-4.580769	10.932128	1.312528
H	-3.562605	12.609952	-0.167127
H	-1.272978	12.262481	-1.076233
H	-0.016887	10.196206	-0.476374
H	-1.027432	8.531306	1.034172
H	-2.734680	2.015965	4.499198
H	-3.947180	-0.108193	4.742574
H	-6.394351	-0.217234	4.305971
H	-7.611051	1.847644	3.626802
H	-6.399901	3.984139	3.419999
H	-2.083978	5.215524	6.462658
H	0.195636	4.545046	7.096428
H	1.659280	3.368893	5.465542
H	0.805349	2.891512	3.174446
H	-1.468986	3.600100	2.527901
H	-6.925691	5.203324	1.460879
H	-9.298726	4.570664	1.029220

H	-9.816251	2.576824	-0.366415
H	-7.958030	1.235238	-1.329565
H	-5.616959	1.862453	-0.894589
H	-1.691071	3.638415	-0.518866
H	-0.261367	1.642022	-0.651901
H	-1.046827	-0.527660	0.281585
H	-3.286947	-0.662176	1.354581
H	-4.735170	1.323615	1.464350
C	-4.543472	5.457361	5.412606
C	-4.518246	4.714858	6.609722
C	-5.241151	5.139753	7.725559
C	-6.019918	6.301925	7.658540
C	-6.078997	7.024927	6.466539
C	-5.345954	6.601470	5.350103
H	-3.957362	3.790865	6.662788
H	-5.208598	4.558680	8.638939
H	-6.585069	6.627273	8.523122
H	-6.693544	7.912787	6.392376
H	-5.421683	7.140345	4.417268
C	-2.249900	8.817634	3.827241
C	-2.041264	10.162776	4.190887
C	-1.050183	10.504575	5.112444
C	-0.236568	9.511010	5.671750
C	-0.415247	8.179544	5.294403
C	-1.415196	7.837841	4.374463
H	-2.634415	10.945286	3.735705
H	-0.903891	11.543120	5.382610
H	0.536353	9.778472	6.381560
H	0.219544	7.403064	5.701320
H	-1.527681	6.813125	4.052518

Cis-Ru(H_2)(dppm)($PPh3)_2$

H	-0.449778	1.235394	-0.057213
H	-0.725465	1.576348	2.397355
C	0.228321	1.779939	1.926651
C	0.379234	1.578921	0.549027
C	1.302550	2.243959	2.690101
H	1.184660	2.403342	3.754636
C	2.533906	2.501475	2.075372
H	3.369742	2.860602	2.662768
C	2.425276	3.184579	-5.505368
C	2.689303	2.289260	0.703592
C	2.254394	3.282870	-2.565229
H	3.314766	3.499349	-2.702725
C	1.610486	1.829843	-0.073091
C	0.570806	4.944101	-4.262800
C	0.708844	5.697402	-5.441188
H	1.196736	5.267900	-6.305870
H	0.354577	7.578127	-6.422809
C	0.237240	7.013349	-5.506141
C	-0.370544	7.599023	-4.393307
H	-0.726133	8.620619	-4.440787
H	-1.011490	7.289398	-2.357149
C	-0.524026	6.854190	-3.219587
C	-0.070104	5.534724	-3.159446
H	-0.237944	4.956243	-2.259702
P	1.183027	3.183058	-4.117070
P	1.790838	1.588570	-1.906975
H	1.289645	1.759558	-6.647717

C	2.165824	2.394939	-6.634694
H	3.650779	2.470264	0.239055
C	3.583729	3.983509	-5.486746
H	3.786452	4.625369	-4.637996
C	4.464239	3.983736	-6.571578
H	5.353045	4.602129	-6.544376
C	4.190631	3.196301	-7.696817
H	4.871522	3.199702	-8.538764
C	3.039451	2.405833	-7.728584
H	2.827551	1.784039	-8.588330
C	3.407421	0.655853	-1.917500
H	2.686729	-0.828461	-0.523527
C	3.521536	-0.505433	-1.130984
C	4.702785	-1.250289	-1.122546
H	4.766385	-2.142748	-0.513453
C	5.795564	-0.847162	-1.897234
H	6.712836	-1.422069	-1.886695
C	5.693584	0.300344	-2.687450
H	6.532022	0.621395	-3.293141
C	4.507202	1.043652	-2.702471
H	4.447376	1.912602	-3.343747
Ru	-0.125871	1.376134	-3.218031
H	-0.847484	0.479405	-2.099835
H	-0.484017	2.530227	-2.157797
P	0.274151	-0.751750	-4.315000
C	0.838966	-2.100408	-3.133596
C	0.387447	-2.079232	-1.803821
H	-0.209622	-1.239140	-1.473015
C	0.714324	-3.110285	-0.915852
H	0.349663	-3.074243	0.103510
C	1.511572	-4.176997	-1.340495
H	1.769242	-4.973946	-0.653926
C	1.973265	-4.207569	-2.660206
H	2.592613	-5.028020	-3.001015
C	1.635319	-3.182629	-3.550082
H	1.993074	-3.228993	-4.569428
C	1.574206	-0.987664	-5.650856
C	1.292660	-1.419707	-6.957313
H	0.277970	-1.652248	-7.247802
C	2.320894	-1.577585	-7.895970
H	2.080044	-1.916115	-8.896417
C	3.647385	-1.321764	-7.541284
H	4.442336	-1.456848	-8.264097
C	3.939589	-0.894309	-6.241765
H	4.962204	-0.692302	-5.949675
C	2.912777	-0.720195	-5.312448
H	3.156516	-0.393103	-4.311978
P	-2.321243	1.928026	-3.855765
C	-3.726967	0.849126	-3.245818
C	-5.041302	1.343472	-3.140870
H	-5.254260	2.371745	-3.402558
C	-6.077112	0.527562	-2.677009
H	-7.080365	0.927934	-2.598617
C	-5.816360	-0.795437	-2.305095
H	-6.618002	-1.426604	-1.942121
C	-4.514214	-1.292969	-2.394488
H	-4.298571	-2.313118	-2.103534
C	-3.478226	-0.474325	-2.857604
H	-2.468751	-0.853579	-2.902646
C	-2.950964	3.545829	-3.143704

H	-4.409934	6.752868	-1.464181
C	-2.923005	3.702060	-1.745543
C	-3.445711	4.847797	-1.143622
H	-2.489814	2.922258	-1.132992
H	-3.421966	4.945313	-0.065195
C	-3.509763	4.569225	-3.922082
H	-4.448992	6.504830	-3.937891
H	-3.543241	4.476520	-4.998404
C	-4.027849	5.722908	-3.318378
C	-4.001925	5.864561	-1.930304
H	1.828867	4.030546	-1.893755
C	-1.147273	-1.664893	-5.127855
C	-1.523152	-2.975905	-4.789200
C	-2.587800	-3.605664	-5.443456
C	-3.287373	-2.941999	-6.454379
C	-2.921983	-1.638174	-6.801298
C	-1.868042	-1.004044	-6.137088
H	-0.990743	-3.510728	-4.015664
H	-2.864180	-4.614542	-5.162700
H	-4.109029	-3.431666	-6.961832
H	-3.458746	-1.106687	-7.576410
H	-1.608082	0.011745	-6.400866
C	-2.780461	2.190064	-5.655514
C	-3.999100	1.793938	-6.230518
C	-4.265489	2.045467	-7.581807
C	-3.322279	2.700321	-8.378995
C	-2.103687	3.096592	-7.818686
C	-1.836244	2.836273	-6.471624
H	-4.736103	1.274305	-5.634974
H	-5.209881	1.728699	-8.007326
H	-3.531795	2.895413	-9.423253
H	-1.362177	3.601728	-8.424816
H	-0.885854	3.125574	-6.044863

Trans-Ru(H_2)(dmpm)$_2$

P	-2.615454	3.275983	0.123364
Ru	-4.302352	4.404035	-0.974085
P	-3.992715	5.477573	1.043614
P	-4.611677	3.330798	-2.992014
P	-5.989424	5.531970	-2.071316
C	-6.069682	4.382556	-3.565250
C	-2.533049	4.427493	1.615604
H	-5.457553	3.391513	-0.287725
H	-3.147045	5.416717	-1.660187
H	-7.001833	3.811538	-3.593355
H	-5.923710	4.876693	-4.530029
H	-1.601367	4.999470	1.639834
H	-2.675769	3.935184	2.581807
C	-5.193733	5.379922	2.462789
H	-5.529752	4.345770	2.550819
H	-4.750087	5.715689	3.404306
H	-6.064697	5.998523	2.233214
C	-3.392622	7.230516	1.222223
H	-4.204019	7.912058	0.955050
H	-3.057914	7.450854	2.239609
H	-2.576150	7.380786	0.514512
C	-2.817494	1.584830	0.874777
H	-2.012537	1.345154	1.575182
H	-3.782491	1.551850	1.382279

H	-2.832084	0.841574	0.073821
C	-0.852693	3.176170	-0.467901
H	-0.172286	2.846870	0.322213
H	-0.796460	2.475983	-1.304966
H	-0.561599	4.163237	-0.829757
C	-7.752557	5.628882	-1.480669
H	-8.433046	5.958448	-2.270607
H	-8.042623	4.641032	-1.120148
H	-7.809883	6.327933	-0.642729
C	-5.789153	7.224475	-2.820178
H	-6.593887	7.463981	-3.520897
H	-5.776287	7.966654	-2.018193
H	-4.823801	7.259566	-3.326883
C	-5.213963	1.578597	-3.170835
H	-6.031263	1.429479	-2.463842
H	-5.548035	1.358582	-4.188502
H	-4.403712	0.896021	-2.902839
C	-3.409605	3.426538	-4.410456
H	-2.539617	2.806796	-4.180263
H	-3.853178	3.091144	-5.352141
H	-3.072148	4.460216	-4.498541

Cis-Ru(H_2)(dmpm)$_2$

P	-0.687398	0.329800	1.639607
Ru	-2.481046	-1.043678	2.262672
P	-2.831526	1.024756	3.215800
P	-1.909610	-2.618606	3.905736
P	-2.308847	-3.092884	1.224911
C	-2.258380	-4.114774	2.803724
C	-1.502027	1.927427	2.236607
H	-4.014300	-1.508925	2.571252
H	-3.224492	-0.396587	0.963212
H	-0.864783	2.621309	2.793369
H	-1.954384	2.451484	1.390141
H	-1.531069	-4.931764	2.843333
H	-3.255706	-4.506311	3.022137
C	-3.684633	-3.808842	0.203684
H	-3.545797	-4.875640	0.009586
H	-4.621456	-3.639113	0.735707
H	-3.731220	-3.267300	-0.743996
C	-0.825712	-3.694805	0.268817
H	-0.886703	-4.764000	0.047138
H	-0.760720	-3.135139	-0.667304
H	0.075175	-3.493441	0.851649
C	-0.198294	-3.003397	4.556200
H	0.505516	-2.973132	3.722121
H	0.092664	-2.233234	5.274877
H	-0.152026	-3.982609	5.041865
C	-2.907956	-2.957723	5.443900
H	-2.681722	-3.937527	5.873353
H	-2.696398	-2.183300	6.185554
H	-3.964806	-2.899749	5.178856
C	-0.221158	0.695295	-0.128531
H	0.391945	1.596261	-0.217521
H	0.330712	-0.156726	-0.533855
H	-1.142205	0.810253	-0.701947
C	1.006015	0.429387	2.431149
H	1.592849	-0.441450	2.128141
H	1.540212	1.340038	2.144539

H	0.889338	0.400204	3.516388
C	-4.393909	1.992192	2.948980
H	-4.658931	1.917926	1.893724
H	-5.193241	1.529316	3.532311
H	-4.287153	3.040164	3.240805
C	-2.448940	1.478949	4.984133
H	-2.471936	2.560722	5.143831
H	-3.184342	1.002864	5.637096
H	-1.460920	1.092811	5.242101

Trans-Ru(H_2)(dhpm)$_2$

P	-2.645202	3.259365	0.139383
Ru	-4.302190	4.404231	-0.974210
P	-4.016472	5.449693	1.055730
P	-4.587774	3.358878	-3.004222
P	-5.959007	5.549249	-2.087861
C	-6.092058	4.360907	-3.547903
C	-2.511657	4.448229	1.598956
H	-5.504607	3.401187	-0.371673
H	-3.099714	5.407331	-1.576619
H	-7.003898	3.764856	-3.488022
H	-6.019961	4.819140	-4.535088
H	-1.600059	5.044558	1.538108
H	-2.582879	3.990430	2.586403
H	-4.993119	2.005791	-3.232656
H	-3.725818	3.457172	-4.142545
H	-1.285105	3.088230	-0.270770
H	-2.773051	1.989989	0.787873
H	-4.878071	5.351001	2.194287
H	-3.611624	6.802941	1.284070
H	-7.319234	5.720069	-1.678001
H	-5.831139	6.818894	-2.735821

Cis-Ru(H_2)(dhpm)$_2$

P	-0.694456	0.322889	1.643028
Ru	-2.519722	-1.040380	2.241061
P	-2.848979	1.028206	3.194340
P	-1.912184	-2.606683	3.892847
P	-2.342734	-3.096879	1.223857
C	-2.256542	-4.116740	2.803822
C	-1.503285	1.929210	2.234800
H	-4.039479	-1.505862	2.541798
H	-3.264456	-0.390631	0.960551
H	-0.870095	2.613636	2.801069
H	-1.941869	2.454680	1.384666
H	-1.516044	-4.917264	2.832548
H	-3.242684	-4.521414	3.038263
H	-2.608855	-2.933257	5.102079
H	-0.611826	-2.938984	4.407336
H	-3.354171	-3.738137	0.444838
H	-1.227422	-3.600245	0.478175
H	-2.564157	1.411051	4.545466
H	-4.005684	1.852183	3.038530
H	-0.243011	0.671216	0.328039
H	0.602686	0.435627	2.251685

Trans-Ru(HCl)(dmpm)$_2$

C	-6.200446	4.244044	-3.432662
P	-5.990374	5.543188	-2.087466
C	-5.667969	7.113901	-3.023574
Ru	-4.314118	4.385822	-0.949888
P	-4.603370	3.339570	-3.013549
C	-3.497920	3.675802	-4.466965
P	-2.610002	3.258948	0.151496
C	-0.848950	3.200116	-0.438440
C	-2.558025	4.393812	1.657186
P	-3.989642	5.474952	1.073782
C	-3.349744	7.212391	1.224735
C	-2.831673	1.560088	0.861089
C	-5.218818	5.396641	2.459992
C	-4.999088	1.541432	-3.231968
C	-7.697993	5.829472	-1.423681
Cl	-6.136115	2.850581	-0.000206
H	-3.200403	5.348612	-1.585200
H	-7.040270	3.599080	-3.159260
H	-6.325064	4.598086	-4.460194
H	-1.617056	4.945277	1.738055
H	-2.753355	3.879754	2.602106
H	-5.635193	4.388326	2.478210
H	-4.764864	5.647480	3.421990
H	-6.035692	6.090913	2.250379
H	-4.146065	7.908098	0.950007
H	-3.013777	7.434343	2.240935
H	-2.525770	7.341058	0.521225
H	-2.094626	1.344770	1.638838
H	-3.846281	1.495003	1.257357
H	-2.738259	0.824741	0.058614
H	-0.169899	2.865616	0.350137
H	-0.780405	2.513805	-1.285686
H	-0.562924	4.195828	-0.780893
H	-8.414216	6.034759	-2.223083
H	-7.985101	4.932848	-0.871611
H	-7.677144	6.675209	-0.732008
H	-6.479812	7.345124	-3.718228
H	-5.557516	7.934839	-2.311535
H	-4.728614	7.012055	-3.568932
H	-5.694171	1.264665	-2.437407
H	-5.435688	1.337402	-4.212766
H	-4.083721	0.956238	-3.115162
H	-2.545627	3.163194	-4.313351
H	-3.945747	3.334421	-5.403893
H	-3.299507	4.747350	-4.517815

Trans-Ru(HCl)(dhpm)$_2$

C	-6.119462	4.320949	-3.494050
P	-5.897352	5.619410	-2.147969
Ru	-4.226562	4.467175	-1.013113
P	-4.518915	3.422884	-3.069844
P	-2.583980	3.302132	0.117246
C	-2.515060	4.435262	1.625021
P	-3.956057	5.501610	1.033760
Cl	-6.081128	2.963084	-0.178497
H	-3.087543	5.422997	-1.607376
H	-6.956686	3.678541	-3.216285
H	-6.237532	4.676476	-4.517644
H	-1.581980	4.998966	1.669568
H	-2.683031	3.933324	2.578277
H	-4.830258	2.046452	-3.278164
H	-3.716976	3.630925	-4.231793
H	-1.211785	3.149663	-0.247750
H	-2.780006	2.009284	0.690213
H	-4.896774	5.398725	2.102760
H	-3.512153	6.834517	1.289906
H	-7.222005	5.853861	-1.673768
H	-5.727394	6.825904	-2.891078

Trans-[Ru(H-H$_2$O(dmpm)$_2$]$^+$

C	-5.553477	4.815968	-3.749436
P	-4.640242	3.348946	-3.010210
C	-5.719772	1.894330	-3.430789
P	-6.003609	5.566176	-2.086534
C	-7.845864	5.341185	-1.982074
C	-5.859224	7.398095	-2.307608
Ru	-4.466940	4.283767	-0.869463
O	-5.969891	2.886546	0.224172
P	-2.585814	3.302658	0.129576
C	-2.695120	1.827518	1.251346
P	-3.937323	5.535260	1.042580
C	-4.795923	5.310118	2.673362
C	-3.182915	3.061907	-4.114157
C	-0.988416	2.999550	-0.753987
C	-2.254355	4.737685	1.296020
C	-3.623013	7.358746	1.021689
H	-3.407240	5.230061	-1.570002
H	-6.382137	4.588310	-4.424683
H	-4.841848	5.467765	-4.263563
H	-1.476846	5.380474	0.874224
H	-1.986232	4.479772	2.323641
H	-4.961479	4.247170	2.856474
H	-4.205529	5.730201	3.491096
H	-5.766015	5.811721	2.645366
H	-4.572890	7.891605	0.943317
H	-3.109834	7.679676	1.930691
H	-3.013975	7.604751	0.150972
H	-1.784259	1.715182	1.843956
H	-3.548680	1.941118	1.921562
H	-2.840972	0.924537	0.653913
H	-0.174408	2.823474	-0.047558
H	-1.091196	2.126632	-1.401962
H	-0.754965	3.866600	-1.373232
H	-8.351138	5.826127	-2.820653
H	-8.087920	4.276565	-1.990564

H	-8.214908	5.775621	-1.050054
H	-6.464019	7.742672	-3.149097
H	-6.195281	7.902286	-1.399095
H	-4.812818	7.652918	-2.479652
H	-6.693612	2.000408	-2.948550
H	-5.867219	1.813109	-4.510381
H	-5.250436	0.975669	-3.070857
H	-2.652334	2.164000	-3.790601
H	-3.494541	2.935024	-5.153052
H	-2.506206	3.913421	-4.034925
H	-6.823248	3.192248	0.541941
H	-6.007221	1.946749	0.029867

Trans-[Ru(H-H_2O(dhpm)$_2$]$^+$

C	-5.616920	4.791323	-3.739004
P	-4.736934	3.316046	-2.972607
Ru	-4.543059	4.255168	-0.843465
O	-6.121844	2.937955	0.187818
P	-6.020688	5.575371	-2.077290
P	-2.678187	3.253815	0.143340
C	-2.290956	4.691124	1.293289
P	-3.961416	5.516640	1.033728
H	-3.452800	5.157916	-1.548715
H	-6.463522	4.567154	-4.387404
H	-4.900929	5.412352	-4.280203
H	-1.499017	5.308298	0.865423
H	-2.032998	4.433272	2.320144
H	-5.577412	2.218064	-3.326646
H	-3.649303	3.033107	-3.843979
H	-1.454714	2.964208	-0.521048
H	-2.705998	2.132120	1.025551
H	-4.569481	5.428644	2.322009
H	-3.692318	6.912899	1.026992
H	-7.445340	5.507206	-2.024571
H	-5.888099	6.976380	-2.281835
H	-6.869792	3.266739	0.693445
H	-6.128576	1.977479	0.165864

Cis-Ru(H_2)(dmpm)($PMet_3$)$_2$

H	-0.607722	0.030961	2.359177
C	-1.504988	-0.583620	2.478032
H	-2.191952	-0.086791	3.167809
H	-2.007195	-0.682975	1.514333
H	1.026645	-3.317403	2.388152
H	0.463382	-2.215455	1.102858
C	0.145308	-2.924992	1.873065
P	-1.101864	-2.287842	3.142674
C	-0.015597	-1.780542	4.574556
H	0.456430	-2.675904	4.982867
H	-0.629814	-1.324118	5.355132
H	0.754062	-1.067491	4.266568
P	-0.948775	-4.345627	1.305359
C	0.185628	-5.800329	1.095339
H	0.590154	-6.057115	2.074742
H	0.995295	-5.592698	0.390969
H	-0.401531	-6.649737	0.738671
H	-1.833725	-3.005692	-0.559742
C	-1.247613	-3.924342	-0.491320

H	-0.302048	-3.789620	-1.024110
H	-1.808938	-4.731731	-0.966941
Ru	-2.417510	-4.241748	3.086333
H	-1.114490	-4.953840	3.767689
H	-2.878023	-5.791809	2.897546
P	-4.440739	-3.766580	1.994274
C	-4.770680	-2.085908	1.238668
H	-3.980382	-1.862243	0.518898
H	-4.739931	-1.329782	2.025857
H	-4.780782	-5.876540	0.818983
H	-5.781837	-4.597693	0.067895
C	-4.806707	-4.831635	0.505370
H	-4.030823	-4.681470	-0.246253
C	-1.845291	-4.659673	6.545412
H	-1.141757	-3.826062	6.522629
H	-2.267457	-4.752522	7.550409
H	-1.303680	-5.569639	6.283527
P	-3.172392	-4.384326	5.267680
C	-4.068819	-2.962234	6.086538
H	-4.298439	-3.176123	7.134631
H	-3.437382	-2.073018	6.028155
H	-4.997020	-2.754911	5.552006
H	-5.739164	-2.045057	0.730940
C	-4.301357	-5.793358	5.724358
C	-6.077845	-3.994372	2.867996
H	-4.501129	-5.819663	6.799521
H	-5.243836	-5.699544	5.184173
H	-3.820914	-6.721974	5.412413
H	-6.916109	-3.793408	2.194567
H	-6.142837	-3.320136	3.723704
H	-6.147621	-5.023315	3.225351

Cis-Ru(H_2)(dhpm)(PH_3)$_2$

H	-0.799247	0.525107	1.666742
H	-2.109064	-0.566199	2.190307
C	-1.711842	0.447400	2.260557
H	-4.108642	1.127199	1.586539
H	-2.612816	2.043437	0.404551
P	-2.889518	1.858002	1.799054
H	-0.027013	0.832383	4.246808
H	-1.937818	0.082904	4.821205
P	-1.400743	1.120837	3.990441
Ru	-2.265640	3.216709	3.628960
H	-0.830804	3.405640	2.886873
H	-1.438669	3.862929	4.855077
P	-4.096093	3.208648	5.069231
H	-3.970833	2.680955	6.393518
H	-5.357067	2.570930	4.807977
P	-2.557260	5.369431	2.908465
H	-1.469727	6.283698	3.021732
H	-2.874113	5.676231	1.546964
H	-3.542894	6.239204	3.482838
H	-4.676148	4.452710	5.479032

Trans-Ru(H_2)(dhpm)$_2$+1Met

C	-6.070450	4.359557	-3.542309
P	-5.935596	5.568910	-2.098520
Ru	-4.293153	4.415949	-0.956380
P	-4.568327	3.364307	-2.983206
P	-2.641906	3.264347	0.151907
C	-2.529917	4.429955	1.631548
P	-4.030915	5.434357	1.089997
H	-5.504827	3.416968	-0.368227
H	-3.078643	5.421390	-1.538785
H	-6.982145	3.764683	-3.469435
H	-6.000872	4.801075	-4.537326
H	-1.619017	5.030676	1.587163
H	-2.608069	3.960014	2.613196
H	-4.969496	2.008644	-3.207682
H	-3.703708	3.455744	-4.121421
C	-0.897458	3.040349	-0.444903
H	-2.820421	1.996324	0.793438
H	-4.906016	5.311452	2.215668
H	-3.637428	6.786395	1.347855
H	-7.299681	5.764104	-1.710336
H	-5.788654	6.825090	-2.769273
H	-0.234093	2.694516	0.350609
H	-0.894777	2.313386	-1.260122
H	-0.553627	3.997872	-0.839081

Trans-Ru(H_2)(dhpm)$_2$+1Phe

C	-5.815011	4.913940	-3.675533
P	-5.611474	5.929700	-2.097941
Ru	-4.342420	4.388119	-0.956176
P	-3.016004	2.883249	0.174022
C	-2.734714	3.956246	1.696618
P	-3.627335	5.450189	0.950541
C	-4.688384	6.132181	2.301780
P	-5.034885	3.373328	-2.911433
H	-3.018749	4.955996	-1.813518
H	-5.674173	3.788863	-0.127753
H	-5.191397	5.309816	-4.478548
H	-6.838935	4.796896	-4.032866
H	-3.276248	3.575235	2.564123
H	-1.689781	4.122725	1.963470
H	-5.189863	7.208899	-2.580496
H	-6.959095	6.312133	-1.803626
H	-2.603661	6.448453	0.994703
H	-1.687127	2.495601	-0.186703
H	-3.402242	1.620063	0.725271
H	-4.213546	2.865937	-3.967785
H	-6.078301	2.403473	-3.048669
C	-6.022808	5.707602	2.402143
C	-6.839091	6.191045	3.429841
C	-6.333240	7.108002	4.357075
C	-5.007403	7.543866	4.255724
C	-4.187742	7.058309	3.232641
H	-6.402962	5.008122	1.665756
H	-7.866984	5.858171	3.501226
H	-6.967725	7.485336	5.149175
H	-4.614551	8.258878	4.967759
H	-3.162892	7.402636	3.157466

Cis-Ru(H_2)(dhpm)$_2$+1Met

C	-2.225230	-4.132543	2.791173
P	-2.310031	-3.109760	1.215190
Ru	-2.517623	-1.060349	2.239878
P	-1.903047	-2.624435	3.889080
P	-0.711078	0.319759	1.638088
C	-1.527674	1.917191	2.242681
P	-2.859874	0.998462	3.204401
H	-4.032752	-1.544654	2.545339
H	-3.276486	-0.402075	0.965429
H	-0.896772	2.603518	2.809380
H	-1.975866	2.443470	1.398105
H	-1.483729	-4.932761	2.821250
H	-3.212928	-4.540957	3.017438
C	-2.821747	-2.981440	5.469855
H	-0.579247	-2.932678	4.359247
H	-3.302063	-3.762516	0.419816
H	-1.178974	-3.592781	0.480027
H	-2.572869	1.385924	4.554914
H	-4.025001	1.813022	3.057673
H	-0.268400	0.678062	0.322500
H	0.589290	0.439563	2.239696
H	-2.559263	-3.954992	5.888389
H	-2.589151	-2.200947	6.197879
H	-3.890613	-2.941588	5.252779

Cis-Ru(H_2)(dhpm)$_2$+1Phe

Ru	-2.769014	-4.239805	2.930936
H	-2.436337	-3.328386	1.632147
H	-2.868753	-2.765538	3.584003
P	-5.042130	-4.004604	2.655640
C	-5.500913	-4.241329	4.463352
P	-3.793316	-4.926204	4.935026
H	-5.717226	-2.804401	2.274934
H	-5.935335	-4.904908	1.989108
H	-5.663601	-3.273518	4.942139
H	-6.344097	-4.902201	4.670311
C	-4.170102	-6.629191	5.570484
P	-1.944112	-5.985898	1.580423
P	-0.483717	-4.299618	3.184561
C	-0.131925	-5.464921	1.749257
H	-1.830023	-7.401643	1.813476
H	-2.099844	-6.115385	0.162149
H	0.253273	-4.906130	4.253226
H	0.412036	-3.205588	2.978026
H	0.174472	-4.895165	0.870388
H	0.584779	-6.266163	1.934772
H	-3.585661	-4.314506	6.213129
C	-4.530468	-6.866564	6.908259
C	-4.823884	-8.162364	7.343716
C	-4.764071	-9.234524	6.446558
C	-4.402499	-9.008699	5.114635
C	-4.100456	-7.713664	4.681433
H	-4.579619	-6.041608	7.609074
H	-5.097307	-8.334580	8.377265
H	-4.991804	-10.237423	6.784877
H	-4.347954	-9.836915	4.419209
H	-3.799111	-7.531704	3.656784

Trans-Ru(HCl)(dhpm)$_2$+1Met

C	-5.963705	4.497933	-3.620332
P	-6.120868	5.460343	-2.011199
H	-6.151722	6.826166	-2.422565
P	-4.855853	3.171859	-2.870851
C	-3.649729	2.686669	-4.188497
H	-5.718725	2.034250	-2.859745
Ru	-4.352692	4.387996	-0.952570
Cl	-2.857149	5.809529	-2.428017
P	-3.858265	5.581258	0.969844
H	-3.121054	6.804452	0.975559
P	-2.606220	3.301101	0.095781
H	-1.245650	3.387737	-0.331677
H	-7.501584	5.313679	-1.681214
H	-4.708440	5.865003	2.082568
C	-2.618875	4.341116	1.669720
H	-2.566994	1.957863	0.581574
H	-5.357334	3.493897	-0.083697
H	-5.360509	5.093141	-4.309482
H	-6.884704	4.174155	-4.106201
H	-3.054201	3.782982	2.500403
H	-1.655577	4.753319	1.971436
H	-4.153418	2.445095	-5.126077
H	-2.966944	3.527025	-4.323537
H	-3.080293	1.819578	-3.847527

Trans-Ru(HCl)(dhpm)$_2$+1Phe

C	-6.163503	4.462155	-3.462340
P	-6.147907	5.526742	-1.902277
Ru	-6.222207	7.548749	-3.030898
P	-5.683736	9.193108	-1.487356
C	-5.503691	10.575554	-2.753924
P	-6.358183	9.602510	-4.123050
P	-6.687369	5.885431	-4.575838
C	-4.846177	4.847200	-0.792086
Cl	-3.769320	7.575871	-3.743367
H	-5.988503	5.644133	-5.797714
H	-7.295786	5.042433	-1.207859
H	-5.659445	9.991971	-5.304905
H	-4.484291	9.273455	-0.718110
H	-7.989531	5.497216	-5.011668
H	-7.556589	10.346135	-4.340396
H	-6.577051	9.751831	-0.525184
H	-7.763110	7.630730	-2.630968
H	-5.130864	4.197314	-3.700184
H	-6.783938	3.565024	-3.455873
H	-5.918522	11.550241	-2.496613
H	-4.446957	10.669502	-3.010233
C	-5.155625	3.910215	0.208711
C	-4.148558	3.410508	1.039419
C	-2.827936	3.841748	0.874591
C	-2.516261	4.776975	-0.117927
C	-3.519394	5.286229	-0.948773
H	-6.177022	3.573986	0.342325
H	-4.393690	2.690550	1.810041
H	-2.048528	3.454066	1.518400
H	-1.495857	5.115517	-0.244823

H	-3.285652	6.019127	-1.713961

Trans-[Ru(H-H_2O(dhpm)$_2$]$^+$ +1Met

C	-2.875931	-0.586489	-0.616857
P	-1.971255	0.809094	0.262630
C	-2.487138	2.395237	-0.529418
P	-1.443669	-1.791169	-0.454974
H	-1.456216	-2.558397	-1.652723
Ru	0.141318	-0.173258	0.101351
P	1.676349	1.583204	0.142425
H	1.526823	2.831360	-0.524482
O	0.315955	-0.753551	2.321051
P	2.218160	-1.011352	-0.584175
H	2.461393	-1.701127	-1.804241
C	3.020858	0.676104	-0.809308
H	0.006481	0.220531	-1.425557
H	-3.828934	-0.901186	-0.191518
H	-3.017137	-0.326101	-1.668299
H	2.991445	0.964622	-1.861457
H	4.037980	0.783652	-0.433249
H	0.196463	-0.147339	3.056592
H	0.561052	-1.625939	2.640025
H	-3.573249	2.494670	-0.537854
H	-2.055480	3.230130	0.025767
H	-2.105329	2.419899	-1.550815
H	-2.676490	0.881271	1.503126
H	-1.953821	-2.785897	0.432327
H	2.366546	2.056211	1.299568
H	3.163091	-1.706645	0.230143

Trans-[Ru(H-H_2O(dhpm)$_2$]$^+$ +1Phe

C	-2.875931	-0.586489	-0.616857
P	-1.972630	0.806973	0.261293
Ru	-2.902132	2.515544	-1.025614
P	-1.364044	4.281678	-0.999597
C	-1.912051	5.013699	-2.644696
P	-3.512121	4.026995	-2.694924
P	-4.113082	0.563332	-1.445685
C	-4.493381	-0.134785	-3.116166
O	-4.298127	3.326285	0.613960
H	-0.601777	0.427304	0.264891
H	-3.710586	3.710796	-4.068112
H	0.047172	4.141228	-1.110304
H	-1.942627	1.943693	-2.146791
H	-3.283396	-1.377336	0.012981
H	-2.221626	-1.026667	-1.372766
H	-1.244122	4.680637	-3.440978
H	-2.009625	6.098320	-2.684709
H	-5.247101	3.440456	0.518023
H	-4.006690	3.638187	1.474575
H	-5.317599	0.256884	-0.740968
H	-2.257757	0.562726	1.638278
H	-4.514902	5.036548	-2.575260
H	-1.384404	5.411578	-0.126470
C	-5.806980	-0.491999	-3.443055
C	-6.094774	-1.020304	-4.707203
C	-5.068969	-1.191395	-5.644461
C	-3.755370	-0.834180	-5.317571

C	-3.467576	-0.305875	-4.053424
H	-6.604909	-0.358916	-2.714002
H	-7.116566	-1.298166	-4.961476
H	-5.292831	-1.602340	-6.627787
H	-2.957441	-0.967264	-6.046624
H	-2.445784	-0.028014	-3.799150

Cis-Ru(H_2)(dhpm)(PH_3)$_2$ +1Met on dhpm

C	-1.719427	0.420934	2.279463
P	-1.410591	1.106038	4.003262
Ru	-2.256967	3.204517	3.619044
P	-2.553991	5.351190	2.891835
P	-2.880767	1.837113	1.796185
P	-4.084139	3.210307	5.058867
H	-0.801673	0.490422	1.690497
H	-2.118561	-0.592815	2.214273
H	-4.111940	1.109780	1.643826
C	-2.536032	2.133460	-0.011098
H	-0.042191	0.802878	4.274081
H	-1.965965	0.083348	4.840722
H	-0.819809	3.383173	2.875733
H	-1.429423	3.870376	4.841324
H	-3.957575	2.698988	6.389725
H	-5.344644	2.566484	4.807308
H	-1.462203	6.263990	2.978477
H	-2.901920	5.667187	1.538621
H	-3.523360	6.224678	3.488473
H	-4.667463	4.457888	5.454416
H	-3.256063	2.859280	-0.395830
H	-1.535290	2.560190	-0.099852
H	-2.602884	1.215264	-0.597542

Cis-Ru(H_2)(dhpm)(PH_3)$_2$ +1Met on PH3

C	-1.719427	0.420934	2.279463
P	-1.410591	1.106038	4.003262
Ru	-2.256967	3.204517	3.619044
P	-2.553991	5.351190	2.891835
P	-2.880767	1.837113	1.796185
P	-4.084139	3.210307	5.058867
H	-0.801673	0.490422	1.690497
H	-2.118561	-0.592815	2.214273
H	-4.111940	1.109780	1.643826
C	-2.536032	2.133460	-0.011098
H	-0.042191	0.802878	4.274081
H	-1.965965	0.083348	4.840722
H	-0.819809	3.383173	2.875733
H	-1.429423	3.870376	4.841324
H	-3.957575	2.698988	6.389725
H	-5.344644	2.566484	4.807308
H	-1.462203	6.263990	2.978477
H	-2.901920	5.667187	1.538621
H	-3.523360	6.224678	3.488473
H	-4.667463	4.457888	5.454416
H	-3.256063	2.859280	-0.395830
H	-1.535290	2.560190	-0.099852
H	-2.602884	1.215264	-0.597542

Cis-Ru(H_2)(dhpm)(PH_3)$_2$ +1Phe on dhpm

C	-1.281157	0.584815	1.919199
P	-1.384673	1.101878	3.744602
C	-2.061280	2.823662	3.720990
P	0.322572	-0.367521	2.152151
Ru	0.823530	0.435476	4.244903
P	0.594981	-1.505757	5.504509
P	1.450969	1.752445	6.008377
H	-1.109353	1.470803	1.304526
H	-2.130967	0.026751	1.521991
H	-2.604935	0.445917	4.124289
H	1.073237	-0.108061	0.966318
H	-0.059996	-1.704954	1.806113
H	1.364402	1.705281	3.384216
H	2.389522	0.039748	4.133843
H	1.097654	-2.750364	5.008146
H	-0.647314	-2.058536	5.970100
H	2.656058	2.507745	5.906600
H	0.636195	2.828161	6.484812
H	1.732011	1.202379	7.302607
H	1.248232	-1.597653	6.775817
C	-1.166006	3.897444	3.576489
C	-1.638910	5.212689	3.546537
C	-3.007985	5.469813	3.675356
C	-3.904606	4.407684	3.831872
C	-3.434656	3.090851	3.852298
H	-0.105320	3.690461	3.493847
H	-0.941199	6.032601	3.431093
H	-3.372888	6.488954	3.658325
H	-4.964556	4.602694	3.936531
H	-4.135238	2.273070	3.971325

Cis-Ru(H_2)(dhpm)(PH_3)$_2$ +1Phe on PH3

C	-1.812613	0.540895	1.941013
P	-1.400114	1.010131	3.728883
Ru	-2.281851	3.196109	3.553495
P	-0.498540	4.688196	3.499605
H	-0.226252	5.381757	2.278026
P	-2.162365	2.319086	1.435885
P	-2.989512	3.753156	5.658914
H	-2.734616	-0.042421	1.913434
H	-1.032280	0.019416	1.385033
H	-0.036317	0.566846	3.809830
H	-1.935574	-0.096141	4.466677
H	-3.255714	2.225424	0.523735
H	-1.151262	2.561913	0.448875
H	-3.740672	2.472462	3.497994
H	-3.163666	4.458864	3.068575
C	1.270495	4.299457	3.929656
H	-4.361810	4.089160	5.846918
H	-2.903703	2.847797	6.765182
H	-2.464040	4.885559	6.364252
H	-0.637516	5.875293	4.291444
C	2.350881	4.919612	3.279847
C	3.666904	4.606024	3.633670
C	3.918538	3.672970	4.645165
C	2.849882	3.049003	5.296339
C	1.533912	3.355470	4.934762
H	2.165349	5.647449	2.499096

H	4.491088	5.088700	3.123375
H	4.937684	3.432076	4.919826
H	3.039363	2.323156	6.077300
H	0.703313	2.859306	5.422731

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A_Phe -1472.134423
Ru    -2.038488    -0.103906    -0.686807
 H    -1.582095    -0.157008    -2.259883
 H    -3.516314    -0.182162    -1.332867
 P     0.288160     0.000235    -0.029316
 C     1.479339    -0.949031    -1.069624
 C     1.222496    -1.119029    -2.436316
 H     0.303475    -0.724026    -2.859008
 C     2.128780    -1.800585    -3.246764
 H     1.913708    -1.926169    -4.304259
 C     3.297870    -2.327498    -2.701269
 H     3.999818    -2.866220    -3.331837
 C     3.560251    -2.166714    -1.341465
 H     4.467298    -2.578898    -0.907916
 C     2.659438    -1.480581    -0.529665
 H     2.873651    -1.364301     0.528263
 C     0.666704    -0.610187     1.670496
 C     1.590524     0.025194     2.511005
 H     2.098995     0.924571     2.177673
 C     1.859811    -0.487189     3.779972
 H     2.573996     0.020247     4.422725
 C     1.217136    -1.641474     4.222311
 H     1.426104    -2.037147     5.212288
 C     0.300660    -2.283941     3.390657
 H    -0.207896    -3.182536     3.728353
 C     0.023877    -1.769377     2.126691
 H    -0.700890    -2.271406     1.492440
 C     0.989306     1.703714    -0.015199
 C     2.114787     2.064346    -0.763168
 C     2.586125     3.377781    -0.736639
 C     1.946822     4.338414     0.042551
 C     0.826679     3.985115     0.796309
 C     0.346439     2.679670     0.761761
 H     2.624539     1.322039    -1.369130
 H     3.457243     3.646290    -1.327909
 H     2.315916     5.359998     0.061464
 H     0.320572     4.728862     1.405333
 H    -0.531918     2.414451     1.345082
 C    -2.121175    -2.000200    -0.934250
 C    -2.840062    -0.019759     1.072034
 C    -2.251168     1.744886    -1.145720
 O    -3.392756     0.038676     2.081879
 O    -2.444197     2.812169    -1.527233
 O    -2.231551    -3.117743    -1.187073
=====================================================
B_Phe -1472.135222
Ru    -0.042641    -0.380617    -2.006549
 H     1.312166    -1.253991    -1.781118
 H     1.075004     0.809647    -2.078029
 P     0.165853     0.071248     0.328254
 C     1.809369    -0.321120     1.060863
 C     2.459029     0.566062     1.926930
 H     2.009128     1.525599     2.160422
 C     3.690453     0.227490     2.488673
 H     4.189173     0.930639     3.149973
 C     4.277564    -1.002329     2.202443
 H     5.237382    -1.263695     2.639377
 C     3.630829    -1.895552     1.347823
 H     4.083452    -2.855717     1.116583
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 C     2.408776    -1.555494     0.775112
 H     1.922731    -2.245062     0.091632
 C    -0.109407     1.832507     0.801922
 H    -0.585037     5.569704     1.776602
 C     0.382059     2.852211    -0.024982
 C     0.216956     4.189223     0.328711
 H     0.886384     2.592953    -0.950957
 H     0.601361     4.967967    -0.323999
 C    -0.772115     2.179520     1.987280
 H    -1.464460     3.773606     3.251866
 H    -1.159803     1.404474     2.640957
 C    -0.942409     3.519278     2.333567
 C    -0.448406     4.526204     1.506571
 C    -1.010316    -0.829848     1.424977
 C    -0.610565    -1.429756     2.625122
 C    -1.542906    -2.085470     3.429481
 C    -2.881779    -2.141508     3.049405
 C    -3.289513    -1.540488     1.858391
 C    -2.359764    -0.894114     1.048864
 H     0.429637    -1.388316     2.932373
 H    -1.218107    -2.553092     4.354877
 H    -3.605747    -2.654482     3.676337
 H    -4.331349    -1.582454     1.553575
 H    -2.683718    -0.437661     0.117530
 C    -1.038387    -2.036886    -1.832609
 C    -1.465622     0.914264    -2.286574
 C     0.425842    -0.598421    -3.829691
 O     0.789509    -0.713905    -4.915674
 O    -2.273760     1.710146    -2.489000
 O    -1.550927    -3.065514    -1.755451
=====================================================
A_met -897.164998
Ru    -0.733920    -0.048463    -0.383131
 H    -0.175889    -0.058278    -1.929329
 H    -2.185126    -0.159461    -1.096385
 P     1.559191     0.093140     0.278731
 C    -0.743432    -1.942698    -0.657548
 C    -1.569139    -0.042973     1.360527
 C    -0.989397     1.807068    -0.779592
 O    -2.110134    -0.039836     2.379089
 O    -1.185467     2.891549    -1.111398
 O    -0.789566    -3.063219    -0.917806
 C     2.722978    -0.873681    -0.766120
 H     2.447902    -1.931461    -0.738076
 H     2.641434    -0.532215    -1.801018
 H     3.756944    -0.761985    -0.424183
 C     2.311703     1.771131     0.240273
 H     2.215981     2.186410    -0.766406
 H     1.778464     2.428469     0.932295
 H     3.370092     1.741032     0.517851
 C     1.988231    -0.485227     1.974138
 H     3.061076    -0.393492     2.173009
 H     1.434477     0.103533     2.710532
 H     1.691336    -1.531549     2.086919
=====================================================
B_met -897.167875
Ru    -2.007192    -0.073420    -0.324067
 H    -1.612162    -1.455032    -1.110144
 H    -1.586229     0.583475    -1.764422
 P     0.335049    -0.017781    -0.070383
 C    -2.363458    -1.129183     1.260913
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 C    -2.328839     1.714899     0.348552
 C    -3.690400    -0.325678    -1.176332
 O    -4.663892    -0.501434    -1.763966
 O    -2.506448     2.798738     0.698366
 O    -2.562298    -1.802991     2.174729
 C     1.247918    -0.531949    -1.575416
 H     0.953398    -1.550082    -1.839792
 H     0.968981     0.124831    -2.402513
 H     2.330234    -0.488975    -1.417426
 C     1.086949     1.615336     0.314209
 H     2.178165     1.547544     0.365704
 H     0.806600     2.331711    -0.462365
 H     0.705178     1.982035     1.270635
 C     1.056951    -1.104477     1.225309
 H     0.756939    -2.138403     1.035849
 H     2.149688    -1.041632     1.232350
 H     0.674931    -0.812745     2.207125
=====================================================
(1   ) FeH2CO4 -211.92406059
Fe     0.000000     0.000000     0.265437
 C     0.000000     1.388904    -0.889109
 C     0.000000    -1.388904    -0.889109
 C    -1.721604     0.000000     0.715873
 C     1.721604     0.000000     0.715873
 H     0.000000     1.004769     1.387696
 H     0.000000    -1.004769     1.387696
 O    -2.792027     0.000000     1.104961
 O     0.000000     2.293313    -1.579830
 O     0.000000    -2.293313    -1.579830
 O     2.792027     0.000000     1.104961
=====================================================
(TS1 ) FeH2CO4 -211.903930173
Fe     0.101846     0.063630     0.223411
 C     0.039830     1.600609    -0.695267
 C    -0.036186    -1.717857     0.356613
 C    -1.689176     0.113658     0.210661
 C     1.694367    -0.228002    -0.544018
 H     0.771502     0.770641     1.534692
 H     0.178989     0.265852     1.842556
 O    -2.830609     0.136779     0.164772
 O    -0.011214     2.560847    -1.312458
 O    -0.130186    -2.855623     0.403476
 O     2.692110    -0.425866    -1.064391
=====================================================
(1a  ) FeH2CO4 -211.911652292
Fe     0.086740     0.106065     0.341056
 C    -0.090308     1.290497    -0.981949
 C    -0.174062    -1.613674    -0.057754
 C    -1.650258     0.300952     0.794835
 C     1.855553    -0.050077     0.012455
 H     0.455855     0.982591     1.602515
 H     0.430570     0.101587     1.883001
 O    -2.742368     0.426922     1.091332
 O    -0.208197     2.036747    -1.840253
 O    -0.343604    -2.711290    -0.329729
 O     2.973040    -0.145121    -0.184202
=====================================================
(TS1a) FeH2CO4 -211.911268329
Fe    -0.000008     0.000155    -0.339209
 C     0.000326    -1.498813     0.642731
 C    -0.000354     1.499163     0.642706
```

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 C    -1.796155    -0.000599    -0.479986
 C     1.796104     0.000048    -0.479962
 H     0.000499    -0.537692    -1.771111
 H    -0.000280     0.540143    -1.770304
 O    -2.927738    -0.001110    -0.602806
 O     0.000601    -2.463527     1.253596
 O    -0.000488     2.464191     1.253064
 O     2.927681    -0.000212    -0.602865
=====================================================
(TS1b) FeH2CO4 -211.892845
Fe     0.153026    -0.080200     0.071196
 C     0.015311    -0.128838     1.835205
 C     1.787876     0.161744    -0.563027
 H     0.626751    -1.403977     0.591566
 H     0.556766     1.356559     0.213236
 C    -1.341176     0.852234    -0.233148
 C    -0.373398    -1.274031    -1.150421
 O    -0.040350    -0.200756     2.973570
 O    -2.280804     1.471208    -0.420445
 O     2.844769     0.362695    -0.946123
 O    -0.694989    -2.055949    -1.916133
=====================================================
(1b  ) FeH2CO4 -211.911508237
Fe     0.044933     0.005899     0.033962
 C     0.245606     0.284693     1.788073
 C     1.812006    -0.019010    -0.234515
 H    -0.192913    -1.392072     0.588398
 H     0.283006     1.403977    -0.520320
 C    -1.612524     0.675617     0.047702
 C    -0.264588    -0.917968    -1.464928
 O     0.358220     0.381139     2.917018
 O    -2.636098     1.173740     0.025595
 O     2.931379     0.043520    -0.433439
 O    -0.470960    -1.575128    -2.371499
=====================================================
(TS1c) FeH2CO4 -211.909935979
 C    -1.794834    -0.007307     0.000360
 O    -2.932156    -0.011265     0.000601
Fe     0.000288    -0.000910     0.000000
 C     0.000235     0.003975     1.794970
 O     0.000138     0.007595     2.932306
 C     1.795429     0.007446    -0.000310
 O     2.932738     0.012953    -0.000508
 C    -0.000422    -0.004458    -1.795046
 O    -0.000984    -0.006282    -2.932377
 H     0.006494    -1.524571     0.003556
 H    -0.005917     1.522775    -0.003552
=====================================================
(2   ) FeHKCO4 -239.694742811
 C     1.282550    -1.439801    -1.016158
 O     1.767341    -2.275544    -1.636562
Fe     0.464194    -0.155311    -0.100217
 C     0.385522     1.375545    -0.927197
 O     0.185056     2.385394    -1.476916
 C     1.778141     0.259949     1.025390
 O     2.618128     0.537414     1.757589
 C    -0.672382    -0.734131     1.086019
 O    -1.537551    -1.050856     1.802398
 H    -0.679075    -0.500093    -1.061623
 K    -2.368943     1.511769     0.155878
=====================================================
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(3   ) MnHCO5 -213.497026584
 C    -1.803443    -0.448763     0.000000
Mn     0.005951    -0.142895     0.000000
 C     1.834587    -0.295884     0.000000
 O     2.962894    -0.453651     0.000000
 O    -2.914027    -0.702905     0.000000
 C     0.015292    -0.372331     1.820622
 O     0.023513    -0.578760     2.941025
 C    -0.069816     1.686297     0.000000
 O    -0.117157     2.826970     0.000000
 C     0.015292    -0.372331    -1.820622
 O     0.023513    -0.578760    -2.941025
 H     0.070525    -1.703310     0.000000
=====================================================
(TS3 ) MnHCO5 -213.460002064
Mn     0.241959    -0.254859     0.139882
 C    -0.034297     0.062866     1.926404
 C     1.769375     0.211079    -0.636929
 C     0.888232    -1.833811     0.783594
 H     0.727166     1.196116     0.283943
 C    -1.297072     0.693497    -0.177677
 C    -0.357520    -1.211439    -1.292134
 O    -0.188248     0.264638     3.039025
 O    -2.245518     1.291990    -0.388847
 O     2.749828     0.557156    -1.121550
 O    -0.748667    -1.793270    -2.193835
 O     1.293434    -2.813488     1.208609
=====================================================
ReHCO5 -645.531909
Re     0.000164    -0.133453    -0.000021
 C     0.000012    -0.319760     1.994910
 O     0.000033    -0.479987     3.131752
 C    -0.000269    -0.320000    -1.994936
 O    -0.000924    -0.480391    -3.131755
 C    -1.994300    -0.323585    -0.000021
 C     1.994678    -0.323457     0.000159
 O    -3.130660    -0.487211    -0.000220
 O     3.130793    -0.488743     0.000315
 C    -0.000241     1.867944    -0.000157
 O    -0.000432     3.020169    -0.000210
 H     0.001094    -1.864800     0.000073
=====================================================
[H3Ru4(C6H6)4(CO)]+
  C        1.93377       -1.71293        2.61904
  C        2.71041       -0.54408        2.46226
  C        2.18875        0.71080        2.86049
  C        0.90918        0.78582        3.47603
  C        0.15365       -0.39219        3.67032
  C        0.64839       -1.63904        3.21850
 Ru        0.73977       -0.22379        1.49885
 Ru        0.47913       -1.19344       -1.08693
 Ru       -1.71530       -0.13063        0.22672
 Ru        0.32794        1.53655       -0.61098
  C        1.36297        3.42525       -0.12384
  C       -0.03624        3.65980       -0.02573
  C       -0.87040        3.39287       -1.13445
  C       -0.33419        2.82542       -2.31263
  C        1.06507        2.59049       -2.40738
  C        1.91185        2.92862       -1.32775
  C       -3.55314        1.04670       -0.07250
  C       -3.58974       -0.07028       -0.94346
```

C	-3.41553	-1.37437	-0.41825
C	-3.21988	-1.56548	0.97238
C	-3.18602	-0.44516	1.83848
C	-3.35703	0.86253	1.31919
C	-0.54550	-2.79285	-2.33229
C	0.03703	-1.82876	-3.18303
C	1.41837	-1.51547	-3.05404
C	2.20545	-2.18083	-2.08524
C	1.60432	-3.09464	-1.19113
C	0.22121	-3.39937	-1.30972
H	-3.28929	1.72101	1.97718
H	-0.24483	-4.08766	-0.61451
H	2.96627	2.68288	-1.37607
H	3.24099	-1.89174	-1.94880
H	-3.04823	-2.56109	1.36462
H	-0.46195	4.03056	0.89921
H	-3.64935	2.04731	-0.47569
H	-1.60283	-3.01464	-2.41584
H	1.48181	2.14201	-3.30120
H	1.86766	-0.76140	-3.68923
H	-3.40576	-2.22856	-1.08426
H	-1.93832	3.55628	-1.05381
H	-3.70268	0.07528	-2.01144
H	-0.57016	-1.31620	-3.91986
H	-0.98849	2.55934	-3.13448
H	-2.99362	-0.58664	2.89529
H	2.19522	-3.54714	-0.40360
H	2.00863	3.61258	0.72634
H	2.75854	1.61279	2.67270
H	-0.83454	-0.32950	4.11010
H	2.30531	-2.66297	2.25331
H	3.65294	-0.58632	1.92969
H	0.50135	1.74643	3.76844
H	0.04320	-2.53265	3.31565
H	-0.72666	0.17982	-1.26685
H	-0.48906	1.01129	0.95646
H	-0.37238	-1.31571	0.54361
C	1.82766	0.15204	-0.27487
O	3.02074	0.24909	-0.42203

==========

[FeH(H2)(DMPE)2]+ -1966.387864

Fe	-0.006368	0.150876	0.068271
P	0.124200	0.098269	2.271251
P	2.214137	-0.118287	0.081414
P	-0.090277	0.920148	-2.015016
P	-2.221079	0.419333	0.055148
C	-2.775579	0.239247	-1.700541
C	-1.866901	1.111226	-2.559045
C	2.793092	-0.316952	1.835207
C	1.869803	0.473169	2.750201
C	0.560200	2.599731	-2.371429
C	0.636002	-0.054957	-3.396341
C	-3.316212	-0.753661	0.946846
C	-2.927478	2.049573	0.512029
C	-0.807388	1.303447	3.293276
C	-0.209560	-1.472783	3.171821
C	2.927490	-1.612833	-0.715369
C	3.321340	1.204979	-0.548448
H	1.717525	-0.150565	-3.265920
H	0.205890	-1.060284	-3.410303
H	0.447439	0.427802	-4.359968

H	1.647841	2.628475	-2.282000
H	0.284602	2.906990	-3.384936
H	0.141346	3.306994	-1.651001
H	4.001864	-1.688645	-0.522297
H	2.433423	-2.506245	-0.324116
H	2.767584	-1.585278	-1.796144
H	4.362192	0.991718	-0.288606
H	3.251475	1.272130	-1.637396
H	3.031191	2.168535	-0.121101
H	-4.366393	-0.588519	0.687438
H	-3.043691	-1.780714	0.688834
H	-3.207263	-0.632082	2.028124
H	-4.003918	2.080831	0.316280
H	-2.754070	2.252768	1.570043
H	-2.431171	2.836932	-0.061434
H	-0.045223	-1.364165	4.248530
H	-1.244662	-1.782395	3.002077
H	0.440622	-2.266152	2.791745
H	-0.446038	1.278688	4.326242
H	-0.670026	2.308944	2.888445
H	-1.874526	1.068284	3.304195
H	-2.129972	2.168393	-2.435618
H	-1.960906	0.883899	-3.625794
H	-2.669971	-0.819218	-1.967749
H	-3.832361	0.505387	-1.817635
H	2.742964	-1.386909	2.071350
H	3.840682	-0.014109	1.937096
H	2.009571	1.551310	2.608298
H	2.042476	0.250305	3.809246
H	0.195767	1.610705	0.393319
H	-0.175395	-1.432246	0.192617
H	-0.214846	-1.262128	-0.657098