Supplementary Material for the paper:-

Five Coordinate Metal Complexes and the Value of τ_5: Observations and Caveats.

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Tables of Cartesian Coordinates.

Cartesian coordinates of optimized species are given below. The following data are listed underneath the coordinates (in Hartree unless otherwise noted):

- Values for β , α and τ
- Imaginary Frequencies
- B3LYP/6-31G(d)-LANL2DZ total potential energy (excluding zero-point energy) at 0 K (E)
- B3LYP/6-31G(d)-LANL2DZ Gibbs free energy at 298.15 K and 1 mol/L (G)

Table 1: hydridotetrakis(triphenylphosphine)rhodium(I)

Rh	15.289529	15.289529	15.289529
H	14.531088	14.531088	14.531088
P	16.769969	16.769969	16.769969
C	17.293817	14.906892	18.753758
C	18.059090	14.285107	19.739959
C	19.386931	14.665466	19.938110
C	19.949498	15.669888	19.147783
C	19.184225	16.291673	18.161582
C	17.856384	15.911314	17.963431
H	16.266619	14.613082	18.601159
H	17.624069	13.510723	20.352634
H	19.979107	14.184893	20.701106
H	20.976696	15.963698	19.300382
H	19.621524	17.068334	17.548908
P	14.071013	13.943467	16.820076
C	12.028006	13.476559	14.963832
C	11.101022	12.706730	14.262331
C	10.932480	11.358391	14.576640
C	11.693198	10.777603	15.594727

C	12.620182	11.547432	16.296228
C	12.788724	12.895771	15.981919
H	12.160106	14.519700	14.720129
H	10.513402	13.155418	13.476559
H	10.212758	10.761660	14.034571
H	11.561098	9.734462	15.838430
H	13.207802	11.098745	17.082000
C	15.947755	12.043949	17.425918
C	16.480714	11.003086	18.159305
C	15.970531	10.634114	19.386931
C	14.852230	11.303729	19.883448
C	14.280552	12.344592	19.150061
C	14.829454	12.715841	17.922434
H	16.371389	12.330926	16.476158
H	17.384921	10.486070	17.774390
H	16.412386	9.827844	19.954054
H	14.428596	11.016751	20.833207
H	13.415064	12.863885	19.532698
C	13.542610	15.829320	18.858528
C	12.809222	16.455660	19.865227
C	11.483659	16.091244	20.095265
C	10.889206	15.098210	19.316326
C	11.620315	14.471870	18.307349
C	12.948156	14.836286	18.079589
H	14.569807	16.111742	18.680875
H	13.269298	17.223211	20.468791
H	10.916537	16.576373	20.876482
H	9.862008	14.815788	19.491701
H	11.160240	13.702042	17.703785
P	16.820076	14.071013	13.943467
P	13.943467	16.820076	14.071013
C	17.963431	17.856384	15.911314

C	15.911314	17.963431	17.856384
C	15.981919	12.788724	12.895771
C	17.922434	14.829454	12.715841
C	18.079589	12.948156	14.836286
C	12.895771	15.981919	12.788724
C	12.715841	17.922434	14.829454
C	14.836286	18.079589	12.948156
C	18.753758	17.293817	14.906892
C	18.161582	19.184225	16.291673
C	14.906892	18.753758	17.293817
C	16.291673	18.161582	19.184225
C	14.963832	12.028006	13.476559
C	16.296228	12.620182	11.547432
C	17.425918	15.947755	12.043949
C	19.150061	14.280552	12.344592
C	18.858528	13.542610	15.829320
C	18.307349	11.620315	14.471870
C	13.476559	14.963832	12.028006
C	11.547432	16.296228	12.620182
C	12.043949	17.425918	15.947755
C	12.344592	19.150061	14.280552
C	15.829320	18.858528	13.542610
C	14.471870	18.307349	11.620315
C	19.739959	18.059090	14.285107
H	18.601159	16.266619	14.613082
C	19.147783	19.949498	15.669888
H	17.548908	19.621524	17.068334
C	14.285107	19.739959	18.059090
H	14.613082	18.601159	16.266619
C	15.669888	19.147783	19.949498
H	17.068334	17.548908	19.621524
C	14.262331	11.101022	12.706730

H	14.720129	12.160106	14.519700
C	15.594727	11.693198	10.777603
H	17.082000	13.207802	11.098745
C	18.159305	16.480714	11.003086
H	16.476158	16.371389	12.330926
C	19.883448	14.852230	11.303729
H	19.532698	13.415064	12.863885
C	19.865227	12.809222	16.455660
H	18.680875	14.569807	16.111742
C	19.316326	10.889206	15.098210
H	17.703785	11.160240	13.702042
C	12.706730	14.262331	11.101022
H	14.519700	14.720129	12.160106
C	10.777603	15.594727	11.693198
H	11.098745	17.082000	13.207802
C	11.003086	18.159305	16.480714
H	12.330926	16.476158	16.371389
C	11.303729	19.883448	14.852230
H	12.863885	19.532698	13.415064
C	16.455660	19.865227	12.809222
H	16.111742	18.680875	14.569807
C	15.098210	19.316326	10.889206
H	13.702042	17.703785	11.160240
C	19.938110	19.386931	14.665466
H	20.352634	17.624069	13.510723
H	19.300382	20.976696	15.963698
C	14.665466	19.938110	19.386931
H	13.510723	20.352634	17.624069
H	15.963698	19.300382	20.976696
C	14.576640	10.932480	11.358391
H	13.476559	10.513402	13.155418
H	15.838430	11.561098	9.734462

C	19.386931	15.970531	10.634114
H	17.774390	17.384921	10.486070
H	20.833207	14.428596	11.016751
C	20.095265	11.483659	16.091244
H	20.468791	13.269298	17.223211
H	19.491701	9.862008	14.815788
C	11.358391	14.576640	10.932480
H	13.155418	13.476559	10.513402
H	9.734462	15.838430	11.561098
C	10.634114	19.386931	15.970531
H	10.486070	17.774390	17.384921
H	11.016751	20.833207	14.428596
C	16.091244	20.095265	11.483659
H	17.223211	20.468791	13.269298
H	14.815788	19.491701	9.862008
H	20.701106	19.979107	14.184893
H	14.184893	20.701106	19.979107
H	14.034571	10.212758	10.761660
H	19.954054	16.412386	9.827844
H	20.876482	10.916537	16.576373
H	10.761660	14.034571	10.212758
H	9.827844	19.954054	16.412386
H	16.576373	20.876482	10.916537
C	10.249200	0.660504	10.818600
H	9.201504	1.161576	10.750272
C	10.727496	-0.569400	10.249200
C	10.818600	1.138800	12.048504
C	11.957400	-1.138800	10.727496
H	10.226424	-0.637728	9.201504
C	12.048504	0.569400	12.526800
H	10.750272	2.186496	12.549576
C	12.526800	-0.660504	11.957400

H 12.025728 -2.186496 10.226424
H 12.549576 0.637728 13.574496
H 13.574496 -1.161576 12.025728
(β = 180.00°, α = 113.90°; τ = 1.10)
0
-4256.5376625
-4255.538418

Table 2: ethynyltetrakis(trimethylphosphine)cobalt(I)

Co -0.000352 -0.000659 0.149292
P 0.004832 0.000659 -2.099159
P 2.229347 -0.305148 0.439528
C -0.004483 -0.000991 2.058503
C -0.006613 -0.000798 3.288430
C 0.954297 1.328917 -2.997909
C 3.513801 -0.589768 -0.895431
C 3.089388 1.081348 1.335939
C 2.725218 -1.724012 1.538551
H -0.009037 -0.001385 4.355047
H 0.982075 1.135108 -4.075522
H 1.976993 1.381950 -2.620211
H 0.482326 2.298103 -2.829989
H 3.483928 0.195337 -1.655129
H 3.339914 -1.551109 -1.386512
H 4.519248 -0.607620 -0.461228
H 4.123279 0.822047 1.590443
H 3.090821 1.977980 0.709546
H 2.531525 1.295315 2.249001
H 2.481904 -2.670325 1.047521
H 3.798011 -1.703153 1.760395

H	2.156584	-1.656061	2.466877
C	0.683874	-1.483592	-2.998537
H	0.507555	-1.408472	-4.076883
H	0.216427	-2.396223	-2.624591
H	1.758179	-1.560195	-2.825136
C	-1.616641	0.157175	-3.004122
H	-1.459208	0.276942	-4.081361
H	-2.175501	1.016320	-2.628917
H	-2.219918	-0.736178	-2.836746
P	-1.380426	-1.778789	0.431478
C	-2.264972	-2.745224	-0.908436
C	-0.613993	-3.219506	1.327469
C	-2.860588	-1.501258	1.526291
H	-1.568137	-3.109935	-1.667265
H	-3.009102	-2.111989	-1.399137
H	-2.784710	-3.608033	-0.478063
H	-1.357773	-3.984184	1.578365
H	0.162576	-3.669445	0.702112
H	-0.151961	-2.845910	2.242683
H	-3.556439	-0.814722	1.036055
H	-3.380591	-2.441124	1.742592
H	-2.519392	-1.046948	2.457432
P	-0.852098	2.083728	0.433788
C	-1.244921	3.335079	-0.904767
C	-2.484903	2.138233	1.326802
C	0.126218	3.224991	1.532295
H	-1.909685	2.915028	-1.663789
H	-0.324497	3.662738	-1.395536
H	-1.731631	4.216553	-0.473558
H	-2.776876	3.164043	1.578391
H	-3.261817	1.691179	0.699763
H	-2.394049	1.550220	2.241596

H	1.067682	3.487866	1.042261
H	-0.429137	4.143587	1.751894
H	0.351011	2.700178	2.461747

(β = 179.98°, α = 118.47°; τ = 1.025)
0
-2067.0988848
-2066.680763

Table 3: tris(1-adamantyloxy)(methyldiazenido)tetrahydrofuranmolybdenum(IV)

Mo	-0.028933	-0.040967	0.471158
O	-0.177229	-0.106932	2.842517
O	-1.928713	-0.212994	0.709298
O	1.055347	-1.571403	0.885299
N	0.192971	0.011214	-1.299072
O	0.732642	1.679694	0.940518
N	0.564739	0.013212	-2.483159
C	-3.122359	-0.285378	-0.070357
C	-4.294534	-0.470722	0.916766
H	-4.125276	-1.381731	1.504128
H	-4.306240	0.372458	1.618484
C	1.049686	-3.287888	-0.866740
H	0.220212	-3.786146	-0.348002
H	0.620110	-2.597022	-1.598990
C	1.878242	-2.491303	0.161403
C	-0.423445	0.331882	-3.522456
H	0.101069	0.360478	-4.479068
H	-0.896903	1.308910	-3.352696
H	-1.213303	-0.429300	-3.582869
C	-3.090272	-1.489687	-1.030871

H	-2.924894	-2.405004	-0.448339
H	-2.243010	-1.386148	-1.717186
C	-4.419422	-1.576562	-1.812966
H	-4.380749	-2.431685	-2.499476
C	3.938209	-2.807329	-1.265096
H	4.754728	-2.283246	-1.777565
C	3.367834	-4.511400	0.499497
H	3.776743	-5.199922	1.250047
C	1.722069	3.819336	1.295543
H	2.388172	3.360534	2.036754
H	0.811840	4.131423	1.823442
C	-3.348842	1.012785	-0.868689
H	-2.508231	1.169102	-1.552955
H	-3.363441	1.860784	-0.172196
C	2.634070	2.303559	-0.485579
H	2.384114	1.543647	-1.232728
H	3.307757	1.840904	0.246920
C	4.520453	-3.783720	-0.222842
H	5.135848	-3.237554	0.504063
H	5.177637	-4.513733	-0.713451
C	-4.629905	-0.275226	-2.615382
H	-5.563364	-0.334634	-3.189927
H	-3.817543	-0.143365	-3.341641
C	2.465387	-3.472006	1.198748
H	1.641856	-3.969466	1.726521
H	3.034420	-2.903089	1.944359
C	1.349072	2.759070	0.236063
C	-0.579525	-1.333055	3.510210
H	0.308625	-1.964520	3.572940
H	-1.332368	-1.833988	2.895350
C	3.036227	-1.771143	-0.557712
H	3.613353	-1.199248	0.180166

H	2.630362	-1.063506	-1.286968
C	-5.630622	-0.558842	0.147934
H	-6.452428	-0.690560	0.863002
C	1.949248	-4.325994	-1.574017
H	1.350646	-4.883668	-2.305566
C	0.387237	3.399848	-0.785067
H	-0.529011	3.712119	-0.267009
H	0.104446	2.654361	-1.534807
C	3.100644	-3.594087	-2.295317
H	3.735429	-4.319183	-2.821621
H	2.696287	-2.909553	-3.051063
C	-0.618194	1.032440	3.612244
H	-1.630826	1.315939	3.293593
H	0.069857	1.847572	3.394026
C	-4.678756	0.927570	-1.649710
H	-4.824491	1.853588	-2.220098
C	2.346923	4.138788	-2.185958
H	2.095123	3.404081	-2.961129
H	2.826991	4.987407	-2.690916
C	1.066308	4.609756	-1.464735
H	0.373789	5.051524	-2.192801
C	1.435491	5.659939	-0.397205
H	1.902463	6.532680	-0.872171
H	0.529629	6.018478	0.109245
C	-1.125329	-0.908826	4.885751
H	-2.220267	-0.912044	4.880083
H	-0.794648	-1.578421	5.684068
C	-0.603136	0.529368	5.050617
H	0.421279	0.529842	5.438355
H	-1.222928	1.136442	5.716272
C	2.533172	-5.300342	-0.530502
H	1.723303	-5.842299	-0.024416

H	3.160044	-6.053129	-1.026191
C	3.316971	3.513473	-1.161481
H	4.225929	3.174803	-1.674470
C	2.403182	5.032606	0.627528
H	2.660307	5.773608	1.395260
C	-5.585508	-1.759822	-0.819679
H	-6.535441	-1.841519	-1.363651
H	-5.458341	-2.693787	-0.256989
C	-5.844137	0.740285	-0.656352
H	-5.902144	1.600353	0.023377
H	-6.798071	0.696063	-1.197641
C	3.683662	4.564977	-0.094508
H	4.389952	4.137763	0.629311
H	4.185829	5.421229	-0.563776

(β = 176.43°, α = 117.38°; τ = 0.984)
0
-1846.3103848
-1845.506750

Table 4: tetracarbonyl(trimethylarsine)iron

As	-0.163932	-0.211111	2.328534
C	0.132281	0.183290	-1.779338
C	0.389262	1.338511	3.380539
C	1.762062	0.284885	0.229650
Fe	0.004276	0.012525	-0.005649
O	0.214835	0.293501	-2.923631
O	2.895654	0.459060	0.398762
C	-1.952073	-0.566214	3.028829
C	0.885202	-1.649451	3.131335
C	-1.138540	1.389283	0.127394

C	-0.630237	-1.661135	-0.129618
O	-1.878091	2.276048	0.230813
O	-1.041437	-2.743228	-0.192452
H	0.737611	-1.669247	4.213366
H	1.937746	-1.476275	2.902636
H	0.562224	-2.595509	2.694532
H	0.271457	1.135452	4.447240
H	-0.231302	2.188388	3.092868
H	1.435390	1.551073	3.155638
H	-1.923847	-0.652486	4.117277
H	-2.605185	0.257758	2.737860
H	-2.313976	-1.497694	2.591196

(β = 179.97°, α = 119.85°; τ = 1.002)
0
-2930.8746367
-2930.773686

Table 5: Dichloridotrimethylniobium

Nb	3.718118	2.146673	3.026572
Cl	3.717369	2.145320	0.669438
Cl	3.718276	2.146856	5.392760
C	1.844778	1.065144	3.100025
H	1.998809	0.125040	3.643755
H	1.467959	0.851336	2.096720
H	1.109694	1.666003	3.649304
C	5.591516	1.065050	3.099421
H	6.326939	1.665533	3.648639
H	5.968138	0.850993	2.096111
H	5.437060	0.125041	3.643209
C	3.717967	4.309874	3.098966
H	2.826650	4.646505	3.642526

H	3.721144	4.742886	2.095567
H	4.605693	4.646507	3.648258

(β = 179.97°, α = 119.89°; τ = 1.001)
0
-1097.2361439
-1097.166285

Table 6: dicarbonyltris(tris(trifluoromethyl)phosphine)iron(0)

Fe	-0.000718	6.134036	-0.079307
P	0.832065	4.130877	-0.060519
C	0.003798	6.137237	1.731681
O	0.006618	6.139450	2.882882
C	-0.008064	6.133185	-1.898855
O	-0.014437	6.134265	-3.048766
C	2.721056	3.947189	-0.334655
F	3.213892	2.725068	-0.089087
F	3.369094	4.817780	0.457432
F	2.985317	4.262732	-1.619514
C	0.706396	3.075384	1.529985
F	0.980241	1.777443	1.335799
F	1.579669	3.560487	2.434046
F	-0.529769	3.166893	2.045782
C	0.242600	2.795251	-1.307314
F	0.056789	3.347168	-2.518023
F	-0.936435	2.307855	-0.880954
F	1.094710	1.770342	-1.450258
P	1.319934	7.854695	-0.068062
P	-2.151714	6.415996	-0.057719
C	0.535935	9.579987	-0.360500
C	2.290160	8.288665	1.522532

C	2.777321	7.997148	-1.309819
C	-3.254923	4.877500	-0.362199
C	-3.007058	7.027760	1.539731
C	-3.008962	7.618638	-1.285622
F	1.346693	10.620383	-0.122065
F	-0.543972	9.711818	0.428170
F	0.133382	9.639816	-1.646769
F	3.276512	9.174684	1.323410
F	1.429402	8.809438	2.418648
F	2.828882	7.178178	2.050466
F	2.399059	7.541077	-2.515641
F	3.788445	7.228220	-0.867093
F	3.236952	9.246238	-1.469239
F	-4.560782	5.057623	-0.119768
F	-2.828719	3.868438	0.415865
F	-3.107501	4.511650	-1.652466
F	-4.270746	7.433072	1.348848
F	-3.017613	6.018901	2.432392
F	-2.316907	8.051628	2.066904
F	-2.421110	7.540612	-2.491193
F	-2.859739	8.873669	-0.825176
F	-4.318398	7.384306	-1.451694

(β = 179.88°, α = 120.03°; τ = 0.9975)
0
-4413.3127386
-4413.244198

Table 7: hydrido-tetrakis(trimethylphosphine)rhodium(I). [$Rh(PMe_3)_4H$]

Rh	0.006996	0.002579	-0.315473
H	0.017563	-0.025622	-1.932856

P	0.001162	0.050348	2.014569
C	-1.616834	-0.114823	2.892827
P	2.164014	0.803759	-0.639000
C	2.925185	0.402055	-2.272381
C	2.463991	2.633415	-0.634990
C	3.569042	0.280983	0.453770
P	-1.800781	1.427355	-0.650205
P	-0.365483	-2.277291	-0.586338
C	0.967242	-1.238563	2.920855
C	0.647690	1.560188	2.862936
C	-1.957758	2.136754	-2.346934
C	-3.523513	0.766242	-0.465277
C	-1.990672	2.993173	0.325832
C	-1.540941	-3.212891	0.502105
C	-1.051204	-2.778383	-2.225714
C	1.074226	-3.443182	-0.515135
H	1.695418	1.714866	2.580057
H	0.581335	1.477919	3.955745
H	0.078520	2.435663	2.530393
H	-2.099545	-1.051189	2.591205
H	-2.275265	0.711550	2.600159
H	-1.495302	-0.104043	3.983854
H	-2.873698	3.569476	0.016611
H	-1.092051	3.605734	0.184789
H	-2.078355	2.763787	1.394883
H	-2.831885	2.795030	-2.442934
H	-2.037238	1.312690	-3.064315
H	-1.047611	2.699006	-2.584069
H	2.946536	-0.686272	-2.398723
H	3.943946	0.802260	-2.365424
H	2.293416	0.817722	-3.064585
H	2.187330	3.049528	0.340700

H	1.812024	3.089892	-1.389267
H	3.509574	2.891478	-0.855628
H	3.653419	-0.812079	0.419150
H	3.372135	0.573303	1.492524
H	4.523123	0.726000	0.139342
H	0.786793	-4.484910	-0.716890
H	1.544561	-3.383116	0.473343
H	1.814975	-3.122320	-1.257098
H	-1.619526	-4.269484	0.211032
H	-2.531450	-2.747092	0.435145
H	-1.212679	-3.161733	1.547493
H	-1.212663	-3.862705	-2.296275
H	-0.354320	-2.458843	-3.007972
H	-2.000008	-2.254933	-2.390362
H	0.575840	-2.230560	2.667324
H	0.915810	-1.102032	4.009004
H	2.013973	-1.199478	2.599331
H	-4.291689	1.520932	-0.685954
H	-3.667380	0.392024	0.555146
H	-3.642873	-0.080888	-1.151333

(β = 179.71°, α = 119.36°; τ = 1.006)
0
-1955.1667715
-1954.765148

Table 8: hydridotetrakis(phosphine)rhodium(I) [$Rh(PH_3)_4H$]

Rh	-0.732375	1.131423	-0.055015
P	1.290550	1.874954	0.784773
H	2.025690	2.918829	0.153535
H	1.402840	2.416555	2.095690

P	-0.852356	2.565522	-1.896204
H	0.176329	3.512404	-2.155098
H	-1.931205	3.479705	-2.044870
P	-2.673786	1.816738	0.999023
H	-3.740832	0.913218	1.262688
H	-3.504143	2.836552	0.452197
P	-0.764376	-0.868306	-1.216967
H	0.300687	-1.806759	-1.120087
H	-0.838957	-0.908545	-2.638707
H	-0.650261	0.155830	1.197733
H	-1.785286	-1.837438	-1.009769
H	2.406499	1.004167	0.928957
H	-0.913874	2.053020	-3.221115
H	-2.659495	2.357850	2.314826

(β = 179.98°, α = 118.26°; τ = 1.028)
0
-1483.8571198
-1483.780168

Table 9: Pentamethylmolybdenum(V)

Mo	0.008102	-0.011093	0.152121
C	1.635745	1.062935	-0.754754
H	1.747937	2.000519	-0.192278
H	1.446320	1.319235	-1.802198
H	2.566436	0.487367	-0.695605
C	-1.717101	-0.973160	-0.694501
H	-1.789245	-1.947650	-0.189363
H	-1.615289	-1.160600	-1.768502
H	-2.635545	-0.402705	-0.519512
C	-1.046357	1.706197	-0.603211
H	-1.980075	1.770175	-0.026673

H -1.311024 1.608561 -1.661049
H -0.467855 2.626205 -0.466380
C 0.108406 -0.105103 2.249264
H -0.314164 -1.051410 2.614716
H -0.457637 0.727282 2.690503
H 1.153663 -0.034892 2.581971
C 0.982801 -1.641026 -0.850915
H 0.410494 -2.570915 -0.759516
H 1.958803 -1.762267 -0.358509
H 1.165934 -1.442067 -1.911979
(β = 131.68°, α = 131.61°; τ = 0.001)
0
-267.7292194
-267.591441

Complex	Functional	d_{calc} / Å	d_{obs} / Å	$\tau_{5(calc)}$	$\tau_{5(obs)}$	$\Delta\tau_{5(calc-obs)}$
ethynyltetrakis(trimethylphosphine)cobalt(I)	B3LYP	0.286	0.265	1.025	1.024	0.001
	M06	0.262	0.265	1.023	1.024	-0.001
(hydrido) tetrakis(triphenylphosphine)rhodium benzene solvate	B3LYP	0.547	0.597	1.081	1.102	-0.021
	M06	0.577	0.597	1.091	1.102	-0.011
tris(1-adamantyloxy)(methyldiazenido)(tetrahydrofuran)molybdenum(IV)	B3LYP	0.374	0.356	0.984	1.019	-0.035
	M06	0.382	0.356	0.999	1.019	-0.020
tetracarbonyl(trimethylarsine)iron	B3LYP	0.082	0.120	1.002	1.008	-0.006
	M06	0.127	0.120	1.008	1.008	0.000
dichloridotrimethylniobium	B3LYP	0.073	0.139	1.001	1.007	-0.006
	M06	0.082	0.139	1.001	1.007	-0.006
dicarbonyltris(tris(trifluoromethyl)phosphine)iron(0)	B3LYP	0.017	0.034	0.997	1.000	-0.003
	M06	0.022	0.034	0.988	1.000	-0.012

Table 10: Comparisons of calculated and observed values of τ_5 using both B3LYP and MO6 functionals for complexes having $\tau_5 > 1$