Supporting Information for:

Pyrazolium- and 1,2-Cyclopentadiene-based Ligands as σ-Donors: a Theoretical Study of Electronic Structure and Bonding

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Table S1. Partitioning of the orbital interaction term according to contributions from all irreducible representations of the molecular point group.[a]

^{MeO}**1**	a		b		ΔE_{orb}
Mo	-142		-43		-184
W	-161		-47		-208
Rh	-284				-284
Ir	-337				-337
Pd	-307		-56		-364
Pt	-358		-69		-427
Ag	-132		-40		-172
Au	-224		-64		-288

^{Me}**3**	a		b		ΔE_{orb}
Mo	-159		-43		-203
W	-176		-47		-224
Rh	-296				-296
Ir	-346				-346
Pd	-322		-59		-381
Pt	-371		-71		-442
Ag	-136		-38		-173
Au	-230		-64		-294

^{Me}**4**	a		b		ΔE_{orb}
Mo	-157		-47		-205
W	-175		-52		-227
Rh	-308				-308
Ir	-347				-347
Pd	-335		-63		-398
Pt	-381		-77		-458
Ag	-137		-41		-178
Au	-233		-70		-303

^{MeO}**4**	a_1 / a / a'	a_2	b_1 / b / a''	b_2	ΔE_{orb}
Mo	-147		-22		-169
W	-172		-25		-196
Rh	-298				-298
Ir	-358				-358
Pd	-323		-61		-385
Pt	-371		-74		-445
Ag	-130	-4	-18	-24	-177
Au	-225	-5	-28	-41	-298

^{Me}**5**	a1 / a / a'	a2	b1 / b / a''	b2	ΔE_{orb}
Mo	-141		-51		-192
W	-157		-47		-205
Rh	-281				-281
Ir	-332				-332
Pd	-300		-67		-367
Pt	-349		-85		-434
Ag	-124	-1	-29	-17	-172
Au	-214	-2	-50	-30	-295

[a] All energies are reported in kJ mol^{-1}.

Table S2. Optimized structures of the studied metal complexes.

^{MeO}1–Mo(CO)$_5$

C	1.047246	-0.215322	2.295897
C	0.000000	0.000000	1.392364
C	-1.047246	0.215322	2.295897
N	-0.648944	0.206160	3.603625
N	0.648944	-0.206160	3.603625
Mo	0.000000	0.000000	-0.940159
C	0.000000	0.000000	-2.921819
O	0.000000	0.000000	-4.070261
O	-2.346648	0.437823	2.181521
C	-3.144743	-0.322481	1.274346
O	2.346648	-0.437823	2.181521
C	3.144743	0.322481	1.274346
C	-1.369298	-1.496340	-1.076325
O	-2.116849	-2.346099	-1.247524
C	-1.417307	1.461001	-0.989974
O	-2.197358	2.292626	-1.077787
C	1.369298	1.496340	-1.076325
O	2.116849	2.346099	-1.247524
C	1.417307	-1.461001	-0.989974
O	2.197358	-2.292626	-1.077787
H	-3.089708	0.079916	0.267480
H	-4.162502	-0.236518	1.649092
H	-2.835888	-1.367104	1.274435
H	-1.262894	-0.171505	4.310842
H	1.262894	0.171505	4.310842
H	2.835888	1.367104	1.274435
H	4.162502	0.236518	1.649092
H	3.089708	-0.079916	0.267480

^{Me}3–Mo(CO)$_5$

C	0.000000	0.000000	-1.463715
C	0.773093	0.775040	-2.337336
N	0.498801	0.449361	-3.620727
N	-0.498801	-0.449361	-3.620727
C	-0.773093	-0.775040	-2.337336
C	1.770723	1.836189	-2.060938
C	-1.770723	-1.836189	-2.060938
Mo	0.000000	0.000000	0.823437
C	0.000000	2.033530	0.857095
O	-0.005880	3.177066	0.913691
C	2.033257	-0.030250	0.857555

O	3.176623	-0.052071	0.913589
C	0.000000	-2.033530	0.857095
O	0.005880	-3.177066	0.913691
C	0.000000	0.000000	2.815767
O	0.000000	0.000000	3.964283
C	-2.033257	0.030250	0.857555
O	-3.176623	0.052071	0.913589
H	-0.712830	-0.972049	-4.453511
H	0.712830	0.972049	-4.453511
H	-1.296947	-2.685956	-1.567193
H	-2.538372	-1.460598	-1.384102
H	-2.256722	-2.189716	-2.972074
H	2.256722	2.189716	-2.972074
H	1.296947	2.685956	-1.567193
H	2.538372	1.460598	-1.384102

^{Me}4–Mo(CO)$_5$

C	-0.019631	-0.754456	3.802237
C	-0.025794	-1.101910	2.357299
C	0.000000	0.000000	1.488821
C	0.025794	1.101910	2.357299
C	0.019631	0.754456	3.802237
C	-0.047064	-2.519136	1.954908
Mo	0.000000	0.000000	-0.805873
C	0.000000	0.000000	-2.799867
O	0.000000	0.000000	-3.947268
C	0.047064	2.519136	1.954908
C	-1.540142	-1.327539	-0.872574
O	-2.410340	-2.065031	-0.967258
C	1.363783	-1.507811	-0.875602
O	2.136553	-2.346385	-0.975302
C	1.540142	1.327539	-0.872574
O	2.410340	2.065031	-0.967258
C	-1.363783	1.507811	-0.875602
O	-2.136553	2.346385	-0.975302
H	-0.906472	-1.169815	4.294425
H	0.836709	-1.217670	4.305628
H	0.906472	1.169815	4.294425
H	-0.836709	1.217670	4.305628
H	-0.194883	-3.193972	2.797386
H	-0.814850	-2.691171	1.198128
H	0.901513	-2.768353	1.467409
H	0.194883	3.193972	2.797386
H	0.814850	2.691171	1.198128

H	-0.901513	2.768353	1.467409

^{MeO}4–Mo(CO)$_5$

C	-0.475942	3.648897	-0.755737
C	0.120888	2.312150	-1.071908
C	0.325977	1.434029	0.000000
C	0.120888	2.312150	1.071908
C	-0.475942	3.648897	0.755737
O	0.377096	2.171554	-2.343782
C	1.199980	1.121039	-2.845163
Mo	-0.085088	-0.925970	0.000000
C	1.276042	-1.568188	-1.363701
O	2.026578	-2.029883	-2.093975
O	0.377096	2.171554	2.343782
C	1.199980	1.121039	2.845163
C	-0.785041	-2.769492	0.000000
O	-1.211020	-3.836107	0.000000
C	1.276042	-1.568188	1.363701
O	2.026578	-2.029883	2.093975
C	-1.464694	-0.528724	1.449074
O	-2.249832	-0.380474	2.266351
C	-1.464694	-0.528724	-1.449074
O	-2.249832	-0.380474	-2.266351
H	0.594243	0.249837	3.080802
H	1.648945	1.516164	3.754125
H	1.964293	0.860259	2.117553
H	0.123572	4.452333	1.188221
H	-1.470709	3.718421	-1.203155
H	0.594243	0.249837	-3.080802
H	1.648945	1.516164	-3.754125
H	1.964293	0.860259	-2.117553
H	-1.470709	3.718421	1.203155
H	0.123572	4.452333	-1.188221

^{Me}5–Mo(CO)$_5$

N	0.001049	-0.030139	-0.002091
C	0.000980	-0.020820	1.372318
C	1.291496	0.020820	1.755193
N	2.040991	0.030139	0.603127
C	1.261276	0.000000	-0.509287
C	3.484428	0.107798	0.619351
Mo	1.908083	0.000000	-2.689409
C	0.658942	1.547833	-3.131135
O	-0.017650	2.418815	-3.431050

C	-1.217688	-0.107798	-0.775690
C	0.484419	-1.357724	-3.215605
O	-0.281978	-2.122224	-3.583228
C	2.475853	0.000000	-4.603132
O	2.801801	0.000000	-5.701769
C	3.196013	-1.547833	-2.378427
O	3.926695	-2.418815	-2.260827
C	3.388365	1.357724	-2.354051
O	4.231247	2.122224	-2.244228
H	1.736104	0.045920	2.734565
H	-0.905805	-0.045920	1.950753
H	3.907271	-0.597416	-0.090855
H	3.824278	1.112054	0.367628
H	3.834589	-0.145382	1.618518
H	-2.056101	0.145382	-0.129154
H	-1.184794	0.597416	-1.601588
H	-1.365269	-1.112054	-1.172026

^{MeO}1–W(CO)$_5$

C	1.049589	-0.213045	2.434322
C	0.000000	0.000000	1.531077
C	-1.049589	0.213045	2.434322
N	-0.649257	0.204049	3.740556
N	0.649257	-0.204049	3.740556
W	0.000000	0.000000	-0.793250
C	1.383049	1.497860	-0.939403
O	2.140990	2.339946	-1.114248
O	-2.347531	0.437622	2.318955
C	-3.150989	-0.324430	1.416525
O	2.347531	-0.437622	2.318955
C	3.150989	0.324430	1.416525
C	-1.424027	1.470428	-0.841052
O	-2.209262	2.299874	-0.924153
C	-1.383049	-1.497860	-0.939403
O	-2.140990	-2.339946	-1.114248
C	1.424027	-1.470428	-0.841052
O	2.209262	-2.299874	-0.924153
C	0.000000	0.000000	-2.792805
O	0.000000	0.000000	-3.942596
H	1.261837	0.170076	4.450856
H	-1.261837	-0.170076	4.450856
H	4.165990	0.240381	1.799054
H	3.104032	-0.079621	0.409822
H	2.840226	1.368310	1.413665

H	-4.165990	-0.240381	1.799054
H	-3.104032	0.079621	0.409822
H	-2.840226	-1.368310	1.413665

^{Me}3–W(CO)$_5$

C	-0.792461	0.756486	-2.475655
C	0.000000	0.000000	-1.601986
C	0.792461	-0.756486	-2.475655
N	0.460497	-0.488520	-3.757970
N	-0.460497	0.488520	-3.757970
W	0.000000	0.000000	0.684453
C	0.000000	2.045387	0.721592
O	0.002392	3.190495	0.777767
C	1.874425	-1.730065	-2.196693
C	-1.874425	1.730065	-2.196693
C	2.045058	0.026239	0.729437
O	3.189567	0.045295	0.795221
C	0.000000	-2.045387	0.721592
O	-0.002392	-3.190495	0.777767
C	-2.045058	-0.026239	0.729437
O	-3.189567	-0.045295	0.795221
C	0.000000	0.000000	2.692843
O	0.000000	0.000000	3.842763
H	-0.986208	0.693088	-4.591144
H	0.986208	-0.693088	-4.591144
H	-2.713713	1.236678	-1.704034
H	-1.514855	2.502994	-1.517015
H	-2.238152	2.211050	-3.106392
H	2.238152	-2.211050	-3.106392
H	2.713713	-1.236678	-1.704034
H	1.514855	-2.502994	-1.517015

^{Me}4–W(CO)$_5$

C	-0.530122	0.537132	-3.933210
C	0.530122	-0.537132	-3.933210
C	0.772498	-0.787585	-2.489431
C	0.000000	0.000000	-1.620805
C	-0.772498	0.787585	-2.489431
C	1.758050	-1.805114	-2.085761
W	0.000000	0.000000	0.671433
C	0.000000	2.044800	0.741394
O	0.007267	3.187060	0.836495
C	-1.758050	1.805114	-2.085761
C	0.000000	0.000000	2.682154

O	0.000000	0.000000	3.830867
C	2.044425	0.044725	0.747651
O	3.185747	0.077341	0.848151
C	0.000000	-2.044800	0.741394
O	-0.007267	-3.187060	0.836495
C	-2.044425	-0.044725	0.747651
O	-3.185747	-0.077341	0.848151
H	1.461058	-0.234146	-4.426156
H	0.221794	-1.460815	-4.436250
H	-1.461058	0.234146	-4.426156
H	-0.221794	1.460815	-4.436250
H	2.300882	-2.224677	-2.931973
H	2.462128	-1.386693	-1.362978
H	1.247474	-2.614727	-1.554225
H	-2.300882	2.224677	-2.931973
H	-2.462128	1.386693	-1.362978
H	-1.247474	2.614727	-1.554225

^{MeO}4–W(CO)$_5$

C	-2.449001	-0.118038	-1.073703
C	-3.789615	0.467214	-0.755514
C	-3.789615	0.467214	0.755514
C	-2.449001	-0.118038	1.073703
C	-1.568011	-0.312659	0.000000
O	-2.308758	-0.370570	2.345497
C	-1.262391	-1.193472	2.856604
W	0.780047	0.068110	0.000000
C	0.398517	1.457002	-1.460179
O	0.259369	2.239991	-2.283369
O	-2.308758	-0.370570	-2.345497
C	-1.262391	-1.193472	-2.856604
C	0.398517	1.457002	1.460179
O	0.259369	2.239991	2.283369
C	1.411664	-1.309120	1.368305
O	1.857946	-2.068521	2.101781
C	2.647167	0.759859	0.000000
O	3.717918	1.178856	0.000000
C	1.411664	-1.309120	-1.368305
O	1.857946	-2.068521	-2.101781
H	-0.388296	-0.590139	-3.087273
H	-1.661967	-1.630508	-3.769351
H	-1.005594	-1.967881	-2.138303
H	-4.588011	-0.138661	-1.188098
H	-3.867360	1.461334	1.203066

H	-0.388296	-0.590139	3.087273
H	-1.661967	-1.630508	3.769351
H	-1.005594	-1.967881	2.138303
H	-3.867360	1.461334	-1.203066
H	-4.588011	-0.138661	1.188098

^{Me}5–W(CO)$_5$

C	0.000000	0.000000	1.639714
N	-1.064963	-0.024096	2.484437
C	-0.673238	-0.016720	3.801226
C	0.673238	0.016720	3.801226
N	1.064963	0.024096	2.484437
C	-2.454086	-0.087081	2.088898
C	2.454086	0.087081	2.088898
W	0.000000	0.000000	-0.631861
C	1.511578	1.378152	-0.730631
O	2.347686	2.149376	-0.859597
C	-1.347171	1.541588	-0.708462
O	-2.093358	2.403608	-0.808802
C	-1.511578	-1.378152	-0.730631
O	-2.347686	-2.149376	-0.859597
C	0.000000	0.000000	-2.645004
O	0.000000	0.000000	-3.792193
C	1.347171	-1.541588	-0.708462
O	2.093358	-2.403608	-0.808802
H	1.377958	0.037026	4.613821
H	-1.377958	-0.037026	4.613821
H	2.662362	-0.653015	1.320753
H	2.706807	1.075787	1.707522
H	3.071563	-0.125415	2.959743
H	-3.071563	0.125415	2.959743
H	-2.662362	0.653015	1.320753
H	-2.706807	-1.075787	1.707522

^{MeO}1–Rh(CO)$_2$Cl

C	-1.993338	1.069733	0.060873
C	-1.110146	-0.006027	0.083055
C	-1.996975	-1.074893	0.039407
N	-3.310574	-0.686763	0.102888
N	-3.302176	0.682368	-0.046928
Rh	0.983916	-0.011449	0.096695
Cl	0.894393	0.230123	-2.242813
O	-1.839637	-2.371607	-0.077642
O	-1.837693	2.367724	0.144825

C	2.863856	-0.010834	-0.003373
O	3.997176	-0.010495	-0.073634
C	0.971811	-0.188008	1.911740
O	0.949392	-0.295594	3.050772
H	-4.006956	1.191250	0.468463
H	-3.979020	-1.178444	-0.474512
C	-0.520780	2.922556	0.066984
C	-0.548975	-2.885801	-0.423387
H	-0.667256	3.999426	0.097566
H	0.082720	2.595415	0.913297
H	-0.041388	2.620444	-0.863897
H	-0.705036	-3.948178	-0.594365
H	-0.175214	-2.395586	-1.322409
H	0.153881	-2.731037	0.394313

^{Me}3–Rh(CO)$_2$Cl

N	-0.037302	0.003536	0.279530
C	-0.092382	-0.161748	1.614872
C	1.202786	-0.328265	2.114935
C	2.010533	-0.283303	0.984262
N	1.239845	-0.141040	-0.121836
C	-1.388097	-0.144435	2.327969
Rh	1.745253	-0.391412	4.113256
C	2.374562	-2.080130	3.886297
O	2.762654	-3.145577	3.718565
C	3.486876	-0.321330	0.863518
Cl	0.862225	1.784390	4.293167
C	2.202778	-0.329977	5.946730
O	2.475364	-0.285844	7.048364
H	-0.790491	-0.058168	-0.384684
H	1.523789	0.209201	-1.021764
H	3.813382	-0.544379	-0.153634
H	3.913787	0.636900	1.167827
H	3.889146	-1.077652	1.536842
H	-2.220632	0.112640	1.671122
H	-1.580444	-1.117829	2.782578
H	-1.319765	0.586167	3.136655

^{Me}4–Rh(CO)$_2$Cl

C	-1.148360	0.156309	0.085894
C	-1.965443	-0.579492	0.945222
C	-3.410918	-0.460405	0.629786
C	-3.441481	0.445002	-0.586099
C	-2.007414	0.750334	-0.831403

Rh	0.912994	0.074627	0.026689
C	2.794521	-0.149521	-0.099977
O	3.917231	-0.294590	-0.180619
C	1.030665	1.717984	0.798382
O	1.082047	2.751719	1.289232
Cl	0.587264	-2.050986	-0.931334
H	-4.009925	1.368557	-0.431134
H	-3.886663	-0.032649	-1.466024
H	-3.833869	-1.453475	0.440285
H	-3.962711	-0.064730	1.489726
C	-1.467964	-1.446674	2.020635
C	-1.575822	1.550207	-1.989339
H	-0.680214	2.125859	-1.752988
H	-1.278854	0.849548	-2.780892
H	-2.364816	2.190893	-2.383962
H	-0.717342	-0.919210	2.614117
H	-2.255432	-1.848281	2.656746
H	-0.919322	-2.267443	1.538298

^{MeO}4–Rh(CO)$_2$Cl

C	-0.123094	-0.154139	-0.134514
C	-0.019531	-0.034458	1.352599
C	1.272641	0.008271	1.872421
C	2.060682	0.004728	0.723168
C	1.326758	-0.126500	-0.573231
O	-1.169389	0.030223	1.955784
C	-1.280957	0.280609	3.362666
Rh	1.875797	0.131439	3.873690
C	1.935067	-1.689632	3.960279
O	1.967788	-2.832934	4.000139
O	3.349032	0.115271	0.588745
C	4.212776	0.383337	1.700762
Cl	1.765053	2.476881	3.649201
C	2.412696	0.349586	5.670032
O	2.734248	0.490002	6.749696
H	-0.647346	-1.074789	-0.400653
H	1.564643	0.717339	-1.224215
H	-2.349492	0.361849	3.547627
H	-0.856259	-0.545124	3.931440
H	-0.767133	1.207089	3.617862
H	5.201570	0.501378	1.263815
H	3.896101	1.295047	2.206737
H	4.201486	-0.450021	2.401569
H	1.647532	-1.030927	-1.095343

H	-0.711464	0.673792	-0.535722

^{Me}5–Rh(CO)$_2$Cl

C	-3.347925	0.395281	-0.515639
C	-3.319643	-0.465327	0.523678
N	-1.997095	-0.651658	0.846154
C	-1.198293	0.069120	0.037260
N	-2.038914	0.713522	-0.794460
C	-1.517717	-1.517819	1.902917
Rh	0.863899	0.074417	0.022155
C	2.753569	-0.055627	-0.056384
O	3.881767	-0.149335	-0.109112
C	-1.623244	1.579589	-1.874444
C	0.903439	1.730377	0.791119
O	0.915691	2.764684	1.278717
Cl	0.712537	-2.065240	-0.916722
H	-4.116901	-0.961419	1.049070
H	-4.173269	0.793778	-1.079244
H	-1.962497	1.177798	-2.829457
H	-2.029599	2.582042	-1.735206
H	-0.536187	1.621986	-1.874387
H	-2.283757	-2.258397	2.125939
H	-0.617287	-2.022856	1.558310
H	-1.297819	-0.942036	2.802527

^{MeO}1–Ir(CO)$_2$Cl

C	-2.166078	1.068709	0.103863
C	-1.279430	-0.007404	0.066919
C	-2.166118	-1.079472	0.017013
N	-3.475834	-0.694024	0.130264
N	-3.474842	0.678008	0.022786
Ir	0.827048	-0.010674	0.067372
Cl	0.683437	0.337766	-2.260232
O	-2.016366	-2.372112	-0.138193
O	-2.018218	2.362890	0.231877
C	2.705117	-0.002878	-0.037428
O	3.842940	0.000856	-0.098267
C	0.854600	-0.274946	1.876563
O	0.858209	-0.439093	3.013668
H	-4.166407	1.170003	0.571349
H	-4.163426	-1.172075	-0.435725
C	-0.715662	2.947862	0.125592
C	-0.747062	-2.891883	-0.550678
H	-0.873805	4.012530	0.278741

H	-0.048510	2.541601	0.885452
H	-0.300050	2.753424	-0.862496
H	-0.919116	-3.952607	-0.716569
H	-0.419177	-2.401585	-1.467031
H	-0.000592	-2.739578	0.227516

^{Me}3–Ir(CO)$_2$Cl

N	-0.043111	-0.008555	0.269415
C	-0.105015	-0.146227	1.607708
C	1.188744	-0.300114	2.116384
C	2.002735	-0.277263	0.986943
N	1.236224	-0.156494	-0.121698
C	-1.406083	-0.128098	2.311368
Ir	1.749608	-0.375082	4.124541
C	2.415414	-2.057318	3.903890
O	2.831572	-3.117766	3.739093
C	3.478923	-0.332431	0.874459
Cl	0.840460	1.793777	4.296374
C	2.226421	-0.329202	5.950627
O	2.518303	-0.305304	7.052065
H	-0.792995	-0.082282	-0.397045
H	1.524016	0.159029	-1.032907
H	3.812218	-0.405616	-0.162019
H	3.920606	0.556507	1.327855
H	3.859034	-1.192885	1.426076
H	-2.230976	0.140974	1.649681
H	-1.608181	-1.105812	2.752583
H	-1.344049	0.591904	3.129178

^{Me}4–Ir(CO)$_2$Cl

C	-1.330473	0.124147	0.073045
C	-2.159915	-0.637139	0.900728
C	-3.602978	-0.466798	0.603921
C	-3.622043	0.510800	-0.554773
C	-2.183757	0.795318	-0.797868
Ir	0.750325	0.047774	0.021006
C	2.629475	-0.156211	-0.100185
O	3.759278	-0.277955	-0.174430
C	0.888897	1.684274	0.817492
O	0.953807	2.715815	1.321694
Cl	0.424055	-2.063411	-0.977344
H	-4.163637	1.437123	-0.334315
H	-4.090565	0.101854	-1.456747
H	-4.049372	-1.437613	0.360147

H	-4.139687	-0.111690	1.490684
C	-1.678836	-1.558572	1.937855
C	-1.747724	1.662829	-1.903787
H	-0.785928	2.125252	-1.682431
H	-1.583225	1.023841	-2.781654
H	-2.496732	2.407862	-2.175491
H	-0.939628	-1.058455	2.568709
H	-2.476918	-1.988227	2.541452
H	-1.118781	-2.355296	1.430332

^{MeO}4–Ir(CO)$_2$Cl

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.515027
C	1.458796	0.000000	1.844370
C	2.329317	-0.052315	0.757536
C	1.458796	-0.000483	-0.329345
O	1.709766	0.066549	3.118251
C	3.041527	0.212050	3.627859
Ir	4.422342	-0.109698	0.757596
C	6.309023	-0.053841	0.759987
O	7.443458	-0.010964	0.762347
O	1.709905	0.065441	-1.603211
C	3.041845	0.210015	-2.112650
C	4.365063	-1.932890	0.759182
O	4.313977	-3.076212	0.760275
Cl	4.378477	2.248656	0.755749
H	-0.483721	-0.874309	1.956460
H	-0.480078	0.880745	-0.431563
H	2.918262	0.323948	4.702504
H	3.634917	-0.672380	3.401189
H	3.512311	1.093460	3.193137
H	2.919003	0.319456	-3.187593
H	3.512214	1.092524	-1.679706
H	3.635395	-0.673741	-1.883705
H	-0.483968	-0.874181	-0.441662
H	-0.480313	0.880623	1.946790

^{Me}5–Ir(CO)$_2$Cl

C	-3.508669	0.442383	-0.509565
C	-3.496351	-0.422990	0.526343
N	-2.178128	-0.644742	0.840570
C	-1.365916	0.061292	0.030355
N	-2.195180	0.729259	-0.795590
C	-1.720272	-1.514388	1.904250

Ir	0.710951	0.045387	0.016954
C	2.597950	-0.083572	-0.057995
O	3.731231	-0.161607	-0.105470
C	-1.765718	1.590792	-1.874876
C	0.783159	1.707345	0.782606
O	0.814819	2.748352	1.265738
Cl	0.514955	-2.095645	-0.927035
H	-4.302897	-0.899458	1.055623
H	-4.326904	0.864125	-1.066528
H	-2.097792	1.186934	-2.831533
H	-2.171213	2.594058	-1.740794
H	-0.678331	1.629123	-1.862872
H	-2.482095	-2.268296	2.095102
H	-0.801638	-2.002487	1.586320
H	-1.536906	-0.943602	2.815121

^{MeO}1–PdCl$_2$(py)

C	-0.523368	1.021447	2.886250
N	0.000000	0.000000	2.204140
C	0.523368	-1.021447	2.886250
C	0.548853	-1.055522	4.269155
C	0.000000	0.000000	4.977204
C	-0.548853	1.055522	4.269155
Pd	0.000000	0.000000	0.062637
Cl	0.000000	2.313711	-0.018431
C	0.000000	0.000000	-1.898140
C	-0.998473	-0.467522	-2.747896
N	-0.629335	-0.243029	-4.028885
N	0.629335	0.243029	-4.028885
C	0.998473	0.467522	-2.747896
C	-2.286171	-1.121137	-2.430149
C	2.286171	1.121137	-2.430149
Cl	0.000000	-2.313711	-0.018431
H	0.909092	-1.835771	2.285893
H	0.991026	-1.905096	4.772974
H	0.000000	0.000000	6.060819
H	-0.991026	1.905096	4.772974
H	-0.909092	1.835771	2.285893
H	-2.954250	-0.404418	-1.948178
H	-2.781284	-1.516305	-3.318827
H	-2.100940	-1.926546	-1.717335
H	2.954250	0.404418	-1.948178
H	2.781284	1.516305	-3.318827
H	2.100940	1.926546	-1.717335

H	0.982494	0.712474	-4.845908
H	-0.982494	-0.712474	-4.845908

^{Me}3–PdCl$_2$(py)

C	-0.523368	1.021447	2.886250
N	0.000000	0.000000	2.204140
C	0.523368	-1.021447	2.886250
C	0.548853	-1.055522	4.269155
C	0.000000	0.000000	4.977204
C	-0.548853	1.055522	4.269155
Pd	0.000000	0.000000	0.062637
Cl	0.000000	2.313711	-0.018431
C	0.000000	0.000000	-1.898140
C	-0.998473	-0.467522	-2.747896
N	-0.629335	-0.243029	-4.028885
N	0.629335	0.243029	-4.028885
C	0.998473	0.467522	-2.747896
C	-2.286171	-1.121137	-2.430149
C	2.286171	1.121137	-2.430149
Cl	0.000000	-2.313711	-0.018431
H	0.909092	-1.835771	2.285893
H	0.991026	-1.905096	4.772974
H	0.000000	0.000000	6.060819
H	-0.991026	1.905096	4.772974
H	-0.909092	1.835771	2.285893
H	-2.954250	-0.404418	-1.948178
H	-2.781284	-1.516305	-3.318827
H	-2.100940	-1.926546	-1.717335
H	2.954250	0.404418	-1.948178
H	2.781284	1.516305	-3.318827
H	2.100940	1.926546	-1.717335
H	0.982494	0.712474	-4.845908
H	-0.982494	-0.712474	-4.845908

^{Me}4–PdCl$_2$(py)

C	0.000000	0.000000	-1.896743
C	1.052001	0.369876	-2.727344
C	0.716140	0.249978	-4.167979
C	-0.716140	-0.249978	-4.167979
C	-1.052001	-0.369876	-2.727344
Pd	0.000000	0.000000	0.056995
H	-0.838978	-1.218540	-4.665971
H	-1.414302	0.430680	-4.667830
H	0.838978	1.218540	-4.665971

H	1.414302	-0.430680	-4.667830
Cl	0.000000	2.312740	-0.049193
Cl	0.000000	-2.312740	-0.049193
N	0.000000	0.000000	2.206543
C	-0.501690	1.032165	2.888670
C	-0.526820	1.066790	4.271534
C	0.000000	0.000000	4.979475
C	0.526820	-1.066790	4.271534
C	0.501690	-1.032165	2.888670
H	-0.871009	1.854615	2.288890
H	-0.950975	1.925365	4.775535
H	0.000000	0.000000	6.063037
H	0.950975	-1.925365	4.775535
H	0.871009	-1.854615	2.288890
C	2.360716	0.839397	-2.254492
H	2.812887	0.065593	-1.625590
H	3.041488	1.107730	-3.060977
H	2.192188	1.691209	-1.584806
C	-2.360716	-0.839397	-2.254492
H	-2.812887	-0.065593	-1.625590
H	-3.041488	-1.107730	-3.060977
H	-2.192188	-1.691209	-1.584806

^{MeO}4–$PdCl_2$(py)

C	-1.111494	0.158654	2.680584
C	-0.037241	-0.059929	1.824872
C	1.042829	-0.213636	2.687347
C	0.717920	-0.101529	4.140724
C	-0.776736	0.156378	4.136046
Pd	-0.043918	-0.134391	-0.147237
Cl	0.434820	2.134383	-0.124830
O	2.296052	-0.441649	2.434392
C	2.787224	-0.578652	1.094265
O	-2.366456	0.367262	2.419635
C	-2.866713	0.402946	1.076344
N	-0.051182	-0.215405	-2.292866
C	-0.249627	0.888943	-3.017671
C	-0.267401	0.876706	-4.400907
C	-0.060569	-0.320089	-5.065395
C	0.151057	-1.463423	-4.313966
C	0.142640	-1.371315	-2.933657
Cl	-0.521914	-2.394894	0.049424
H	1.296912	0.707891	4.591011
H	-1.352464	-0.616635	4.649992

H	0.272871	-2.240368	-2.300652
H	0.317832	-2.424792	-4.781940
H	-0.064235	-0.360972	-6.148149
H	-0.437581	1.800092	-4.938905
H	-0.375797	1.803288	-2.451135
H	3.851413	-0.772266	1.207200
H	2.291813	-1.414474	0.600893
H	2.616498	0.343338	0.539481
H	-3.930164	0.604797	1.181550
H	-2.374863	1.199058	0.518011
H	-2.699507	-0.558297	0.591523
H	-1.053897	1.113089	4.584438
H	0.998351	-1.021776	4.658098

^{Me}5–PdCl$_2$(py)

N	-0.006659	1.069689	-2.730579
C	0.000000	0.000000	-1.918697
N	0.006659	-1.069689	-2.730579
C	0.002087	-0.675017	-4.047684
C	-0.002087	0.675017	-4.047684
Pd	0.000000	0.000000	0.029596
Cl	2.209243	-0.662983	-0.072113
C	0.000000	-2.441466	-2.269735
C	0.000000	2.441466	-2.269735
N	0.000000	0.000000	2.156360
C	-1.129573	-0.208332	2.837962
C	-1.168765	-0.222986	4.220430
C	0.000000	0.000000	4.928194
C	1.168765	0.222986	4.220430
C	1.129573	0.208332	2.837962
Cl	-2.209243	0.662983	-0.072113
H	2.021040	0.344433	2.239146
H	2.109443	0.402749	4.724060
H	0.000000	0.000000	6.011679
H	-2.109443	-0.402749	4.724060
H	-2.021040	-0.344433	2.239146
H	-0.988047	-2.710377	-1.895932
H	0.263305	-3.091710	-3.101950
H	0.735087	-2.549389	-1.473854
H	0.988047	2.710377	-1.895932
H	-0.263305	3.091710	-3.101950
H	-0.735087	2.549389	-1.473854
H	-0.002465	1.380552	-4.859633
H	0.002465	-1.380552	-4.859633

^{MeO}1–$PtCl_2$(py)

C	-0.285879	1.113511	-2.996801
N	0.000000	0.000000	-2.313046
C	0.285879	-1.113511	-2.996801
C	0.302684	-1.150205	-4.378511
C	0.000000	0.000000	-5.087134
C	-0.302684	1.150205	-4.378511
Pt	0.000000	0.000000	-0.210394
Cl	-0.792715	-2.175732	-0.175632
C	0.000000	0.000000	1.780756
C	1.047953	-0.249012	2.664435
N	0.646654	-0.239587	3.975401
N	-0.646654	0.239587	3.975401
C	-1.047953	0.249012	2.664435
O	2.329721	-0.471764	2.519523
O	-2.329721	0.471764	2.519523
Cl	0.792715	2.175732	-0.175632
H	1.263986	0.193335	4.648833
H	-1.263986	-0.193335	4.648833
C	2.920780	-0.449272	1.216049
C	-2.920780	0.449272	1.216049
H	0.480292	-1.993367	-2.398508
H	0.546742	-2.076549	-4.881586
H	0.000000	0.000000	-6.170481
H	-0.546742	2.076549	-4.881586
H	-0.480292	1.993367	-2.398508
H	3.970540	-0.678462	1.384340
H	2.457761	-1.204099	0.581271
H	2.800853	0.534137	0.763476
H	-3.970540	0.678462	1.384340
H	-2.457761	1.204099	0.581271
H	-2.800853	-0.534137	0.763476

^{Me}3–$PtCl_2$(py)

C	-0.686339	0.921966	2.846338
N	0.000000	0.000000	2.163677
C	0.686339	-0.921966	2.846338
C	0.716125	-0.949955	4.228241
C	0.000000	0.000000	4.936544
C	-0.716125	0.949955	4.228241
Pt	0.000000	0.000000	0.055000
Cl	0.000000	2.314672	0.031645
C	0.000000	0.000000	-1.919243
C	-0.983734	-0.497153	-2.774931

N	-0.622031	-0.261283	-4.055847
N	0.622031	0.261283	-4.055847
C	0.983734	0.497153	-2.774931
C	-2.254350	-1.185184	-2.459625
C	2.254350	1.185184	-2.459625
Cl	0.000000	-2.314672	0.031645
H	1.201361	-1.660595	2.247045
H	1.293185	-1.714308	4.731844
H	0.000000	0.000000	6.019962
H	-1.293185	1.714308	4.731844
H	-1.201361	1.660595	2.247045
H	-2.946925	-0.483077	-1.990854
H	-2.730047	-1.604297	-3.348162
H	-2.055106	-1.976997	-1.735992
H	2.946925	0.483077	-1.990854
H	2.730047	1.604297	-3.348162
H	2.055106	1.976997	-1.735992
H	0.957670	0.746728	-4.870811
H	-0.957670	-0.746728	-4.870811

^{Me}4–$PtCl_2$(py)

C	0.000000	0.000000	-1.919637
C	1.027113	0.432322	-2.758500
C	0.698947	0.294399	-4.198314
C	-0.698947	-0.294399	-4.198314
C	-1.027113	-0.432322	-2.758500
Pt	0.000000	0.000000	0.048255
H	-0.759777	-1.268401	-4.696923
H	-1.438418	0.340359	-4.699448
H	0.759777	1.268401	-4.696923
H	1.438418	-0.340359	-4.699448
Cl	0.000000	2.314025	0.013870
Cl	0.000000	-2.314025	0.013870
N	0.000000	0.000000	2.168480
C	-0.663752	0.938136	2.851161
C	-0.692654	0.967312	4.233068
C	0.000000	0.000000	4.941249
C	0.692654	-0.967312	4.233068
C	0.663752	-0.938136	2.851161
H	-1.161696	1.689213	2.252666
H	-1.250627	1.745638	4.736747
H	0.000000	0.000000	6.024644
H	1.250627	-1.745638	4.736747
H	1.161696	-1.689213	2.252666

C	2.309375	0.976961	-2.292433
H	2.794752	0.245727	-1.638672
H	2.979103	1.258664	-3.103903
H	2.099522	1.836939	-1.644959
C	-2.309375	-0.976961	-2.292433
H	-2.794752	-0.245727	-1.638672
H	-2.979103	-1.258664	-3.103903
H	-2.099522	-1.836939	-1.644959

^{MeO}4–$PtCl_2$(py)

C	-1.111836	0.154479	2.673526
C	-0.037299	-0.060531	1.809079
C	1.043115	-0.210017	2.679992
C	0.718229	-0.094380	4.132645
C	-0.777106	0.148630	4.128533
Pt	-0.044023	-0.135524	-0.177079
Cl	0.711843	2.054942	-0.220901
O	2.299484	-0.441477	2.443784
C	2.834267	-0.584447	1.121925
O	-2.369833	0.367789	2.429037
C	-2.913579	0.410811	1.103808
N	-0.051171	-0.215237	-2.288231
C	-0.332645	0.872945	-3.013060
C	-0.353454	0.858002	-4.395231
C	-0.060559	-0.319933	-5.061065
C	0.237132	-1.444380	-4.310298
C	0.225673	-1.355049	-2.930826
Cl	-0.799609	-2.322865	-0.050487
H	1.289233	0.724531	4.576171
H	-1.344888	-0.634359	4.636398
H	0.417738	-2.213280	-2.300950
H	0.473627	-2.390661	-4.778689
H	-0.064225	-0.360808	-6.143624
H	-0.593353	1.766328	-4.932036
H	-0.520666	1.776279	-2.448411
H	3.874505	-0.863622	1.275153
H	2.296622	-1.361931	0.580493
H	2.756394	0.359662	0.585296
H	-3.952828	0.701011	1.242578
H	-2.379805	1.145116	0.501665
H	-2.839095	-0.571096	0.639385
H	-1.066338	1.098444	4.583741
H	1.010776	-1.007238	4.656215

^{Me}5–$PtCl_2$(py)

N	-0.017079	1.070353	-2.754214
C	0.000000	0.000000	-1.935097
N	0.017079	-1.070353	-2.754214
C	0.007893	-0.674662	-4.070262
C	-0.007893	0.674662	-4.070262
Pt	0.000000	0.000000	0.021042
Cl	2.167066	-0.806602	0.003333
C	0.000000	-2.446376	-2.306782
C	0.000000	2.446376	-2.306782
N	0.000000	0.000000	2.123383
C	-1.098821	-0.340331	2.804762
C	-1.134563	-0.359108	4.186264
C	0.000000	0.000000	4.893885
C	1.134563	0.359108	4.186264
C	1.098821	0.340331	2.804762
Cl	-2.167066	0.806602	0.003333
H	1.967050	0.580472	2.206448
H	2.047259	0.648643	4.689908
H	0.000000	0.000000	5.977205
H	-2.047259	-0.648643	4.689908
H	-1.967050	-0.580472	2.206448
H	-1.011691	-2.744727	-2.030403
H	0.358151	-3.081210	-3.115603
H	0.658165	-2.546145	-1.446306
H	1.011691	2.744727	-2.030403
H	-0.358151	3.081210	-3.115603
H	-0.658165	2.546145	-1.446306
H	-0.012658	1.379828	-4.882536
H	0.012658	-1.379828	-4.882536

^{MeO}1–AgCl

C	0.000000	0.000000	0.896619
C	-1.066822	0.053044	1.786174
N	-0.679161	0.115896	3.099040
N	0.679161	-0.115896	3.099040
C	1.066822	-0.053044	1.786174
O	-2.369184	0.035263	1.624422
O	2.369184	-0.035263	1.624422
Ag	0.000000	0.000000	-1.184742
Cl	0.000000	0.000000	-3.480109
C	-2.901103	-0.045743	0.301148
H	-1.212823	-0.387737	3.794037
H	1.212823	0.387737	3.794037

C	2.901103	0.045743	0.301148
H	3.980050	0.071921	0.429645
H	2.609312	-0.826678	-0.282785
H	2.553744	0.950327	-0.197647
H	-3.980050	-0.071921	0.429645
H	-2.609312	0.826678	-0.282785
H	-2.553744	-0.950327	-0.197647

^{Me}3–AgCl

C	0.000000	0.000000	-0.997021
C	-0.052413	1.094966	-1.860420
N	0.000000	0.672580	-3.143252
N	0.000000	-0.672580	-3.143252
C	0.052413	-1.094966	-1.860420
H	-0.224760	1.180579	-3.982557
H	0.224760	-1.180579	-3.982557
Ag	0.000000	0.000000	1.071545
Cl	0.000000	0.000000	3.369205
C	-0.176422	2.539666	-1.552820
H	-1.215417	2.792948	-1.328719
H	0.407110	2.765849	-0.661173
H	0.165919	3.171958	-2.373823
C	0.176422	-2.539666	-1.552820
H	1.215417	-2.792948	-1.328719
H	-0.407110	-2.765849	-0.661173
H	-0.165919	-3.171958	-2.373823

^{Me}4–AgCl

C	0.004471	0.757764	-3.298724
C	0.007564	1.105693	-1.852145
C	0.000000	0.000000	-1.001034
C	-0.007564	-1.105693	-1.852145
C	-0.004471	-0.757764	-3.298724
Ag	0.000000	0.000000	1.069728
Cl	0.000000	0.000000	3.363760
H	-0.858384	1.200838	-3.808210
H	0.885288	1.186734	-3.789234
H	0.858384	-1.200838	-3.808210
H	-0.885288	-1.186734	-3.789234
C	0.000000	-2.507666	-1.401759
C	0.000000	2.507666	-1.401759
H	-0.427470	-3.191986	-2.135664
H	1.044473	-2.807379	-1.244143
H	-0.493640	-2.606141	-0.434453

H	0.427470	3.191986	-2.135664
H	-1.044473	2.807379	-1.244143
H	0.493640	2.606141	-0.434453

^{MeO}4–AgCl

C	1.082235	0.000000	1.844542
C	0.000000	0.000000	0.969193
C	-1.082235	0.000000	1.844542
C	-0.758276	0.000000	3.305988
C	0.758276	0.000000	3.305988
Ag	0.000000	0.000000	-1.116435
Cl	0.000000	0.000000	-3.412823
O	-2.358155	0.000000	1.584066
C	-2.850927	0.000000	0.240627
O	2.358155	0.000000	1.584066
C	2.850927	0.000000	0.240627
H	-1.195376	-0.876785	3.788963
H	1.195376	0.876785	3.788963
H	3.933670	0.000000	0.337104
H	2.514197	-0.889893	-0.289727
H	2.514197	0.889893	-0.289727
H	-3.933670	0.000000	0.337104
H	-2.514197	0.889893	-0.289727
H	-2.514197	-0.889893	-0.289727
H	-1.195376	0.876785	3.788963
H	1.195376	-0.876785	3.788963

^{Me}5–AgCl

N	0.000000	1.065652	-1.875560
C	0.000000	0.000000	-1.047253
N	0.000000	-1.065652	-1.875560
C	0.000000	-0.674970	-3.193384
C	0.000000	0.674970	-3.193384
Ag	0.000000	0.000000	1.018952
Cl	0.000000	0.000000	3.302292
H	0.000000	1.378108	-4.008264
H	0.000000	-1.378108	-4.008264
C	0.000000	2.443290	-1.437030
H	0.000000	2.455863	-0.349391
H	0.890256	2.956854	-1.802011
H	-0.890256	2.956854	-1.802011
C	0.000000	-2.443290	-1.437030
H	0.000000	-2.455863	-0.349391
H	-0.890256	-2.956854	-1.802011

H	0.890256	-2.956854	-1.802011

^{MeO}1–AuCl

C	0.000000	0.000000	-1.073798
C	0.039370	-1.073979	-1.961943
N	0.107657	-0.680450	-3.271734
N	-0.107657	0.680451	-3.271733
C	-0.039370	1.073979	-1.961943
O	0.002954	-2.374459	-1.808229
O	-0.002954	2.374460	-1.808228
Au	0.000000	0.000000	0.937145
Cl	0.000000	-0.000001	3.213098
C	-0.096414	-2.934240	-0.495459
H	-0.408768	-1.206318	-3.963379
H	0.408768	1.206320	-3.963379
C	0.096414	2.934240	-0.495458
H	-0.130153	-4.009447	-0.651843
H	0.770460	-2.659144	0.103490
H	-1.001676	-2.587490	0.001298
H	0.130153	4.009447	-0.651841
H	-0.770460	2.659143	0.103491
H	1.001676	2.587490	0.001299

^{Me}3–AuCl

C	-0.025336	1.099879	-2.044123
C	0.000000	0.000000	-1.182275
C	0.025336	-1.099879	-2.044123
N	0.052299	-0.670992	-3.324575
N	-0.052299	0.670992	-3.324575
Au	0.000000	0.000000	0.815509
Cl	0.000000	0.000000	3.093433
C	0.000000	-2.546496	-1.730023
C	0.000000	2.546496	-1.730023
H	-0.161536	-1.194655	-4.156905
H	0.161536	1.194655	-4.156905
H	0.627110	-2.731540	-0.858406
H	-1.012750	-2.859185	-1.465323
H	0.349978	-3.159357	-2.562409
H	-0.627110	2.731540	-0.858406
H	1.012750	2.859185	-1.465323
H	-0.349978	3.159357	-2.562409

^{Me}4–AuCl

C	-0.006373	0.758021	-3.475621
C	-0.007776	1.110381	-2.033502
C	0.000000	0.000000	-1.184700
C	0.007776	-1.110381	-2.033502
C	0.006373	-0.758021	-3.475621
Au	0.000000	0.000000	0.811775
Cl	0.000000	0.000000	3.088071
H	-0.887756	1.183835	-3.968332
H	0.855745	1.202190	-3.985836
H	0.887756	-1.183835	-3.968332
H	-0.855745	-1.202190	-3.985836
C	0.000000	-2.508225	-1.575230
C	0.000000	2.508225	-1.575230
H	0.345660	-3.209180	-2.335141
H	0.571512	-2.608177	-0.650977
H	-1.032119	-2.774790	-1.313217
H	-0.571512	2.608177	-0.650977
H	1.032119	2.774790	-1.313217
H	-0.345660	3.209180	-2.335141

^{MeO}4–AuCl

C	0.757824	0.000000	3.283938
C	1.089281	0.000000	1.826525
C	0.000000	0.000000	0.952757
C	-1.089280	0.000000	1.826525
C	-0.757823	0.000000	3.283939
O	2.364727	0.000000	1.575929
C	2.894047	0.000000	0.244647
Au	0.000000	0.000000	-1.059050
Cl	-0.000001	0.000000	-3.337507
O	-2.364726	0.000000	1.575930
C	-2.894047	0.000000	0.244648
H	-1.194096	-0.876738	3.767979
H	1.194097	0.876738	3.767978
H	3.973394	0.000000	0.375457
H	2.568508	-0.887857	-0.294893
H	2.568508	0.887857	-0.294893
H	-3.973394	0.000000	0.375458
H	-2.568508	0.887857	-0.294892
H	-2.568508	-0.887857	-0.294892
H	-1.194096	0.876738	3.767979
H	1.194097	-0.876738	3.767978

^{Me}5–AuCl

C	0.000000	0.000000	-1.073798
C	0.039370	-1.073979	-1.961943
N	0.107657	-0.680450	-3.271734
N	-0.107657	0.680451	-3.271733
C	-0.039370	1.073979	-1.961943
O	0.002954	-2.374459	-1.808229
O	-0.002954	2.374460	-1.808228
Au	0.000000	0.000000	0.937145
Cl	0.000000	-0.000001	3.213098
C	-0.096414	-2.934240	-0.495459
H	-0.408768	-1.206318	-3.963379
H	0.408768	1.206320	-3.963379
C	0.096414	2.934240	-0.495458
H	-0.130153	-4.009447	-0.651843
H	0.770460	-2.659144	0.103490
H	-1.001676	-2.587490	0.001298
H	0.130153	4.009447	-0.651841
H	-0.770460	2.659143	0.103491
H	1.001676	2.587490	0.001299