Supporting Information For

Heterobimetallic Dioxygen Activation: Synthesis and Reactivity of Mixed Cu-Pd and Cu-Pt Bis(μ-oxo) Complexes

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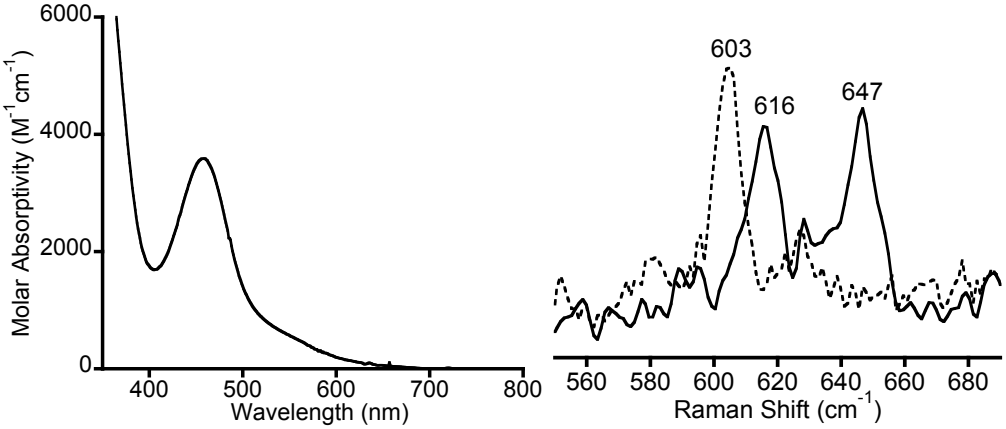

Figure S1. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(Me_4chd)Cu(\mu\text{-}O)_2Pt(PPh_3)_2]PF_6$ in CH_2Cl_2.

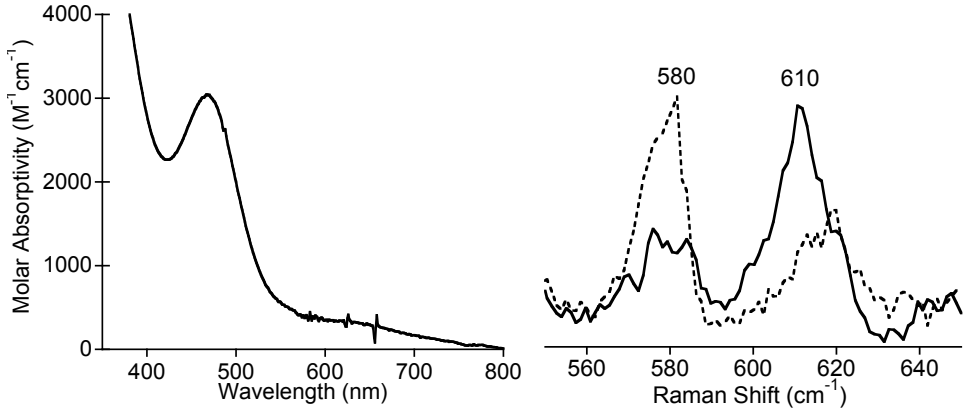

Figure S2. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(Me_4pda)Cu(\mu\text{-}O)_2Pd(PPh_3)_2]CF_3SO_3$ in CH_2Cl_2.

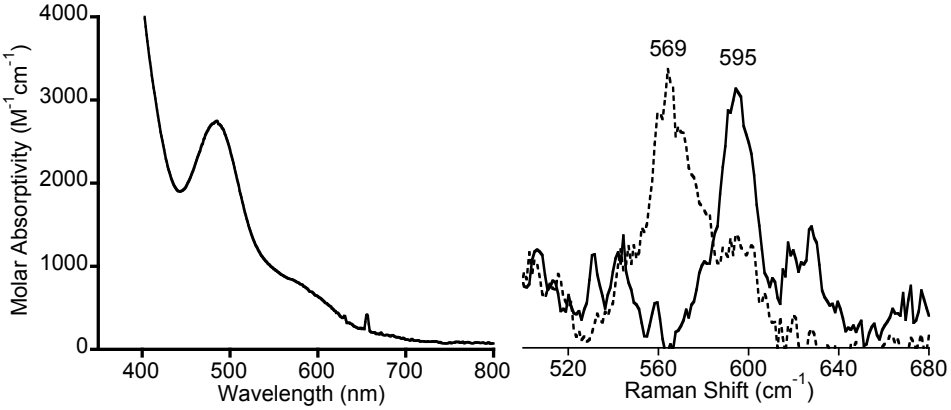

Figure S3. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(Me_4pda)Cu(\mu\text{-}O)_2Pt(PPh_3)_2]$ CF_3SO_3 in CH_2Cl_2.

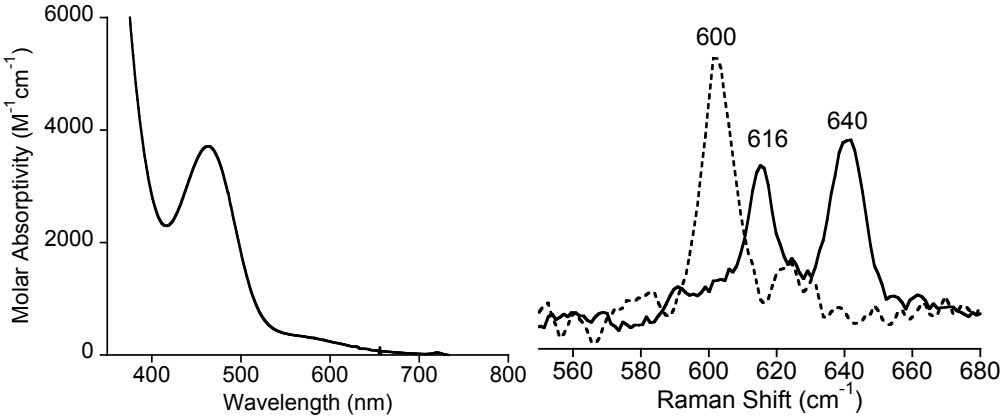

Figure S4. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(Me_4chd)Cu(\mu\text{-}O)_2Pd(PPh_3)_2]PF_6$ in CH_2Cl_2.

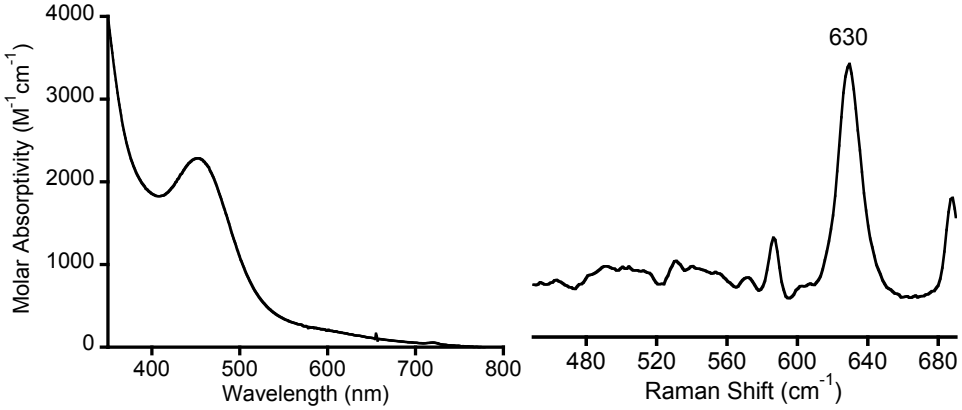

Figure S5. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(iPr_3tacn)Cu(\mu\text{-}O)_2Pd(PPh_3)_2]SbF_6$ in CH_2Cl_2.

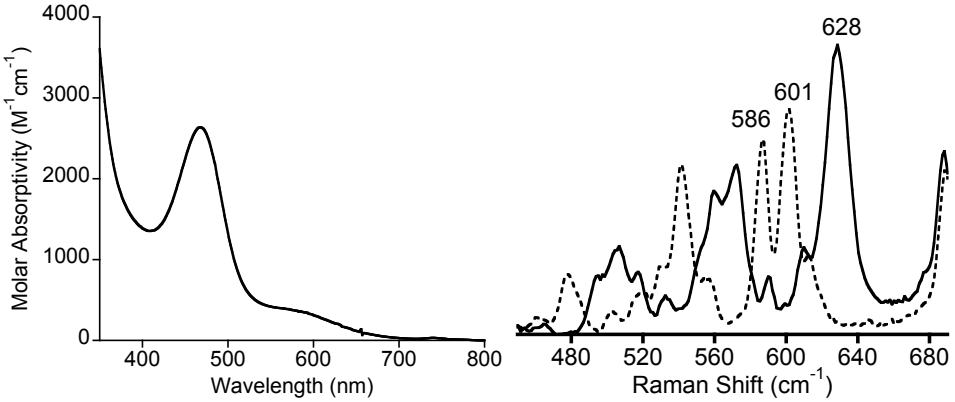

Figure S6. (left) UV-vis spectrum (-80 °C) and (right) resonance Raman spectra (-196 °C, ^{16}O solid line, ^{18}O dashed line) of $[(iPr_3tacn)Cu(\mu\text{-}O)_2Pt(PPh_3)_2]SbF_6$ in CH_2Cl_2.

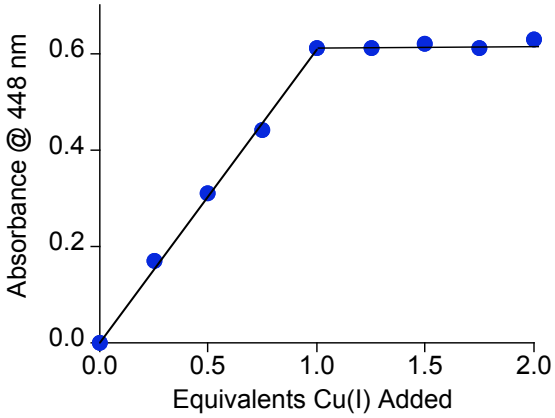

Figure S7. Plot showing results of spectrophotometric titration of $(PPh_3)_2PdO_2$ with $[(L^{Me2})Cu(NCCH_3)]$ in THF at –80 °C. Reproduced from the supporting information in ref. 1.

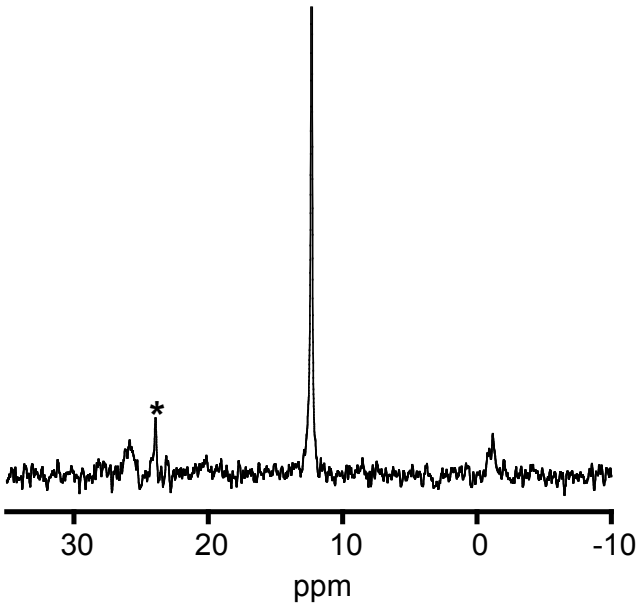

Figure S8. $^{31}P\{^1H\}$ NMR spectrum of $L^{Me2}Cu(\mu\text{-}O)_2Pt(PPh_3)_2$ in THF at -80 °C (* denotes $OPPh_3$).

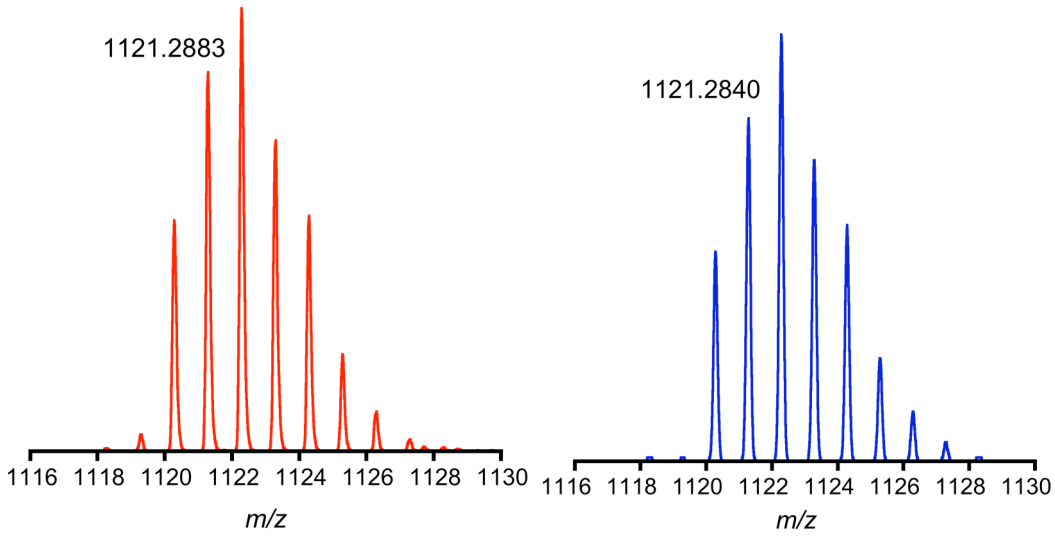

Figure S9. Experimental (left, red) and calculated (right, blue) isotope pattern for the parent ion of $[PtCuP_2N_2C_{57}H_{57}O_2]^+$, the product of the reaction of $L^{Me2}Cu(\mu\text{-}O)_2Pt(PPh_3)_2$ with $[NH_4][PF_6]$.

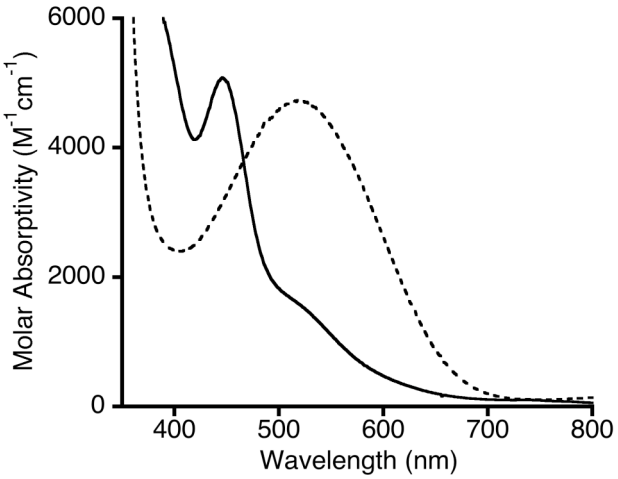

Figure S10. UV-vis spectrum (-80 °C) of $L^{Me2}Cu(\mu\text{-}O)_2Pt(PPh_3)_2$ in CH_2Cl_2 (solid line) and of the solution resulting immediately after reaction with CO_2 (dashed line). The latter absorption featured decayed rapidly (several min).

Complete reference 38: *Gaussian 03*, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.;

Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

Table S1. Selected experimental and calculated bond distances and angles for [Cu^{III}(H33m)].

	Exp	Calc
Cu-C	1.901	1.914
Cu-N(trans)[a]	2.002	2.067
Cu-N(cis)	1.952	1.996
Cu-N(cis)	1.960	1.996
C-Cu-N(trans)	178.37	178.25
C-Cu-N(cis)	81.69	82.61
C-Cu-N(cis)	82.79	82.61
N(trans)-Cu-N(cis)	99.73	97.19
N(trans)-Cu-N(cis)	95.63	97.19
N(cis)-Cu-N(cis)	157.24	160.18

[a] cis and trans is referred to the Cu-C bond.

Cartesian coordinates for all theoretical structures.

1

O	0.000000	1.196275	0.000000
O	0.000000	-1.196275	0.000000
Cu	0.000000	0.000000	1.354954
Cu	0.000000	0.000000	-1.354954
N	0.000000	1.352829	2.650314
N	0.000000	-1.352829	2.650314
N	0.000000	1.352829	-2.650314
N	0.000000	-1.352829	-2.650314
C	0.000000	1.222039	3.959563
C	0.000000	-1.222039	3.959563
C	0.000000	1.222039	-3.959563
C	0.000000	-1.222039	-3.959563
H	0.000000	2.291734	2.265107
H	0.000000	-2.291734	2.265107
H	0.000000	2.291734	-2.265107
H	0.000000	-2.291734	-2.265107
H	0.000000	2.141829	4.551397
H	0.000000	-2.141829	4.551397
H	0.000000	2.141829	-4.551397
H	0.000000	-2.141829	-4.551397
C	0.000000	0.000000	4.644915
C	0.000000	0.000000	-4.644915
H	0.000000	0.000000	5.728343
H	0.000000	0.000000	-5.728343

2

Cu	-0.000071	1.362334	0.000000
Pd	0.000032	-1.472657	0.000000
O	-0.000065	0.059668	1.265456
O	-0.000065	0.059668	-1.265456
N	-0.000076	2.671146	1.347712
N	-0.000076	2.671146	-1.347712
C	-0.000076	3.979707	1.221562
C	-0.000076	3.979707	-1.221562
C	-0.000075	4.667806	0.000000
H	-0.000075	2.274991	2.282287
H	-0.000075	2.274991	-2.282287
P	0.000119	-2.866932	1.828256
P	0.000119	-2.866932	-1.828256
H	-0.000076	5.751327	0.000000
H	-0.000076	4.570522	2.142643
H	-0.000076	4.570522	-2.142643
H	1.059607	-3.759363	2.107802
H	1.059607	-3.759363	-2.107802
H	-1.059312	-3.759418	2.107842
H	0.000122	-2.138175	-3.031630
H	0.000122	-2.138175	3.031630
H	-1.059312	-3.759418	-2.107842

3

Cu	-0.000013	-1.626633	0.000000
Pt	0.000032	1.242743	0.000000
O	0.000032	-0.321591	1.264604
O	0.000032	-0.321591	-1.264604
N	-0.000061	-2.934067	1.345658
N	-0.000061	-2.934067	-1.345658
C	-0.000120	-4.242732	1.221028
C	-0.000120	-4.242732	-1.221028
C	-0.000153	-4.931450	0.000000
H	-0.000041	-2.533958	2.278768
H	-0.000041	-2.533958	-2.278768
P	0.000032	2.652885	1.773715
P	0.000032	2.652885	-1.773715
H	-0.000202	-6.014929	0.000000
H	-0.000145	-4.831991	2.142956
H	-0.000145	-4.831991	-2.142956
H	-1.063359	3.551278	2.016458
H	-1.063359	3.551278	-2.016458
H	1.063439	3.551254	2.016474
H	0.000015	1.958753	-2.998170
H	0.000015	1.958753	2.998170
H	1.063439	3.551254	-2.016474

4

O	0.000000	1.230765	0.000000
O	0.000000	-1.230765	0.000000
Cu	0.000000	0.000000	1.398417
Cu	0.000000	0.000000	-1.398417
N	0.000000	1.391042	2.763321
N	0.000000	-1.391042	2.763321
N	0.000000	1.391042	-2.763321
N	0.000000	-1.391042	-2.763321
C	0.000000	1.237087	4.066444
C	0.000000	-1.237087	4.066444
C	0.000000	1.237087	-4.066444
C	0.000000	-1.237087	-4.066444
H	0.000000	2.345200	2.419943
H	0.000000	-2.345200	2.419943
H	0.000000	2.345200	-2.419943
H	0.000000	-2.345200	-2.419943
H	0.000000	2.139208	4.695674
H	0.000000	-2.139208	4.695674
H	0.000000	2.139208	-4.695674
H	0.000000	-2.139208	-4.695674
C	0.000000	0.000000	4.740640
C	0.000000	0.000000	-4.740640
H	0.000000	0.000000	5.826914
H	0.000000	0.000000	-5.826914

5

Cu	-1.274144	-0.000002	-0.000026
Pd	1.576870	-0.000002	-0.000044
O	0.129374	1.357227	-0.000252
O	0.129369	-1.357226	0.000216
N	-2.712208	1.391548	0.000132
N	-2.712208	-1.391551	-0.000132
C	-4.016011	1.238206	0.000132
C	-4.016011	-1.238212	-0.000066
C	-4.689416	-0.000003	0.000044
H	-2.382410	2.352152	0.000188
H	-2.382407	-2.352154	-0.000178
P	2.640559	2.018532	0.000049
P	2.640579	-2.018522	0.000054
H	-5.776281	-0.000002	0.000071
H	-4.651193	2.137842	0.000214
H	-4.651192	-2.137847	-0.000102
H	4.040455	2.348789	-0.000309
H	4.040482	-2.348737	0.000157
H	2.296998	2.877201	-1.063093
H	2.297293	-2.877018	-1.063289
H	2.297575	2.876778	1.063707
H	2.297351	-2.876952	1.063511

6

Cu	-1.609543	0.000000	-0.000042
Pt	1.300464	0.000000	-0.000039
O	-0.186796	-1.329041	-0.000028
O	-0.186796	1.329041	-0.000250
N	-3.044396	-1.393132	-0.000150
N	-3.044397	1.393131	0.000207
C	-4.348197	-1.238529	-0.000065
C	-4.348198	1.238527	0.000213
C	-5.020924	-0.000001	0.000099
H	-2.716832	-2.354542	-0.000245
H	-2.716834	2.354542	0.000273
P	2.571490	-1.865641	0.000183
P	2.571484	1.865643	0.000019
H	-6.107782	-0.000002	0.000137
H	-4.984102	-2.137627	-0.000130
H	-4.984103	2.137625	0.000322
H	3.998897	-1.927104	-0.000286
H	3.998892	1.927121	0.000940
H	2.380942	-2.785340	1.058173
H	2.379977	2.785759	1.057446
H	2.380088	-2.785845	-1.057181
H	2.381028	2.785439	-1.057901

7

O	-1.399766	-0.067542	0.000000
O	1.085541	0.111850	0.000000
Cu	-0.078649	-0.020550	1.381703
Cu	-0.078649	-0.020550	-1.381703
N	-1.311900	0.021395	2.787991
N	1.359747	-0.167554	2.512793
N	-1.311900	0.021395	-2.787991
N	1.359747	-0.167554	-2.512793
C	-1.043793	0.009317	4.081340
C	1.369041	0.058641	3.812686
C	-1.043793	0.009317	-4.081340
C	1.369041	0.058641	-3.812686
H	-2.260956	-0.241370	2.531334
H	2.231019	-0.084895	1.993672
H	-2.260956	-0.241370	-2.531334
H	2.231019	-0.084895	-1.993672
H	-1.893076	-0.092428	4.760243
H	2.354361	0.171004	4.270469
H	-1.893076	-0.092428	-4.760243
H	2.354361	0.171004	-4.270469
C	0.237777	0.117434	4.629428
C	0.237777	0.117434	-4.629428
H	0.357655	0.205129	5.701886
H	0.357655	0.205129	-5.701886
H	-1.928749	0.744066	0.000000

8

Cu	1.396845	-0.101236	-0.131274
Pd	-1.467969	-0.032991	-0.082741
O	0.066078	-1.466870	-0.284930
O	0.090195	1.129885	-0.410091
N	2.776915	-1.362283	-0.028121
N	2.535021	1.299600	0.208330
C	4.058042	-1.139919	0.193519
C	3.854158	1.278062	0.219956
C	4.644869	0.128315	0.251424
H	2.451737	-2.318454	0.091189
H	2.051240	2.185489	0.085600
P	-3.200434	-1.547125	0.305186
P	-2.575614	1.941436	0.113420
H	5.719156	0.220258	0.348405
H	4.694827	-2.015978	0.334691
H	4.345507	2.253522	0.234720
H	-4.238657	-1.671369	-0.636453
H	-3.976567	2.045049	0.044667
H	-3.963888	-1.441164	1.482211
H	-2.171433	2.871262	-0.854518
H	-2.784385	-2.886634	0.399654
H	-2.318637	2.635600	1.306088
H	0.073742	-1.802896	-1.193006

9

Cu	1.661853	-0.087367	-0.129197
Pt	-1.239070	-0.012278	-0.066589
O	0.307141	-1.443717	-0.303717
O	0.354918	1.138873	-0.421895
N	3.042818	-1.349838	-0.026826
N	2.791585	1.313541	0.231102
C	4.322593	-1.124157	0.198642
C	4.110907	1.294317	0.235673
C	4.904720	0.146593	0.261291
H	2.722895	-2.307895	0.092758
H	2.304268	2.196819	0.101911
P	-2.891250	-1.560868	0.341717
P	-2.462353	1.862545	0.143172
H	5.978827	0.241739	0.357602
H	4.962850	-1.997664	0.339951
H	4.599968	2.271000	0.250380
H	-3.924403	-1.742367	-0.596464
H	-3.562975	2.040778	-0.711652
H	-3.650641	-1.474298	1.523037
H	-1.695008	3.009922	-0.104621
H	-2.402396	-2.874423	0.446696
H	-3.043162	2.149575	1.390152
H	0.300969	-1.754708	-1.221102

10

O	0.116933	-1.413775	0.114192
O	0.094782	1.104200	0.110700
Cu	1.429255	-0.073878	0.047986
Cu	-1.427780	-0.027946	0.030019
N	2.863191	-1.322124	-0.014313
N	2.581869	1.369464	-0.067531
N	-2.828175	-1.362823	-0.095894
N	-2.706257	1.434778	0.034832
C	4.153384	-1.058923	-0.084360
C	3.895331	1.369151	-0.090426
C	-4.129636	-1.132000	-0.140310
C	-4.017301	1.333200	-0.012674
H	2.599452	-2.299722	-0.082135
H	2.069267	2.245489	-0.062235
H	-2.576956	-2.342950	-0.179365
H	-2.341536	2.380706	0.079069
H	4.838141	-1.909949	-0.142637
H	4.381406	2.348262	-0.118652
H	-4.794795	-1.998185	-0.227751
H	-4.601730	2.260212	0.004278
C	4.706822	0.226936	-0.094491
C	-4.738158	0.128642	-0.089083
H	5.783275	0.342785	-0.131956
H	-5.821145	0.179063	-0.126640
H	0.131063	-1.813308	0.995164

11

Cu	-1.391282	-0.082252	-0.067780
Pd	1.562885	-0.032004	-0.055833
O	0.098190	-1.512946	-0.205299
O	0.047242	1.195957	-0.171312
N	-2.758313	-1.457668	0.100203
N	-2.736452	1.326553	-0.039930
C	-4.064613	-1.278882	0.181644
C	-4.041737	1.185960	0.046043
C	-4.720964	-0.040820	0.146100
H	-2.457627	-2.424672	0.173528
H	-2.398443	2.281934	-0.095486
P	3.305447	-1.549515	0.150964
P	2.287006	2.093057	0.126097
H	-5.803656	-0.027752	0.214120
H	-4.694308	-2.169627	0.288627
H	-4.655996	2.094145	0.043785
H	3.263643	-2.417984	1.262167
H	3.648995	2.482476	0.265358
H	4.660343	-1.165941	0.261394
H	1.759455	2.801024	1.213441
H	3.477843	-2.534499	-0.846728
H	1.941850	2.916244	-0.952437
H	0.089350	-1.874825	-1.101463

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Cu	-1.691856	-0.052941	-0.075734
Pt	1.309275	-0.024145	-0.047502
O	-0.168373	-1.484001	-0.232184
O	-0.240558	1.185726	-0.206136
N	-3.053674	-1.430387	0.097495
N	-3.033224	1.357599	-0.024356
C	-4.359269	-1.248964	0.195697
C	-4.336778	1.217696	0.076445
C	-5.014737	-0.010499	0.176809
H	-2.757721	-2.399633	0.160565
H	-2.691461	2.311730	-0.079386
P	3.003315	-1.545980	0.191825
P	2.252332	1.996036	0.152982
H	-6.096544	0.002218	0.257900
H	-4.989145	-2.139410	0.303561
H	-4.951119	2.125835	0.087354
H	3.853255	-1.506918	1.321154
H	1.811104	2.749963	1.250812
H	4.016994	-1.704950	-0.782768
H	1.968270	2.869446	-0.905910
H	2.603438	-2.894760	0.287734
H	3.646175	2.207988	0.272702
H	-0.163176	-1.807421	-1.143502

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Cu	-1.907095	-0.273520	-0.046666
Cu	0.727635	-1.292340	-0.058930
O	-0.161818	0.346286	-0.322232
O	-0.994257	-1.816434	0.197787
N	-2.784096	1.390731	-0.347613
N	-3.523193	-1.164537	0.301200
C	-4.081380	1.621963	-0.280013
C	-4.738642	-0.665882	0.299907
C	-5.061503	0.671865	0.030714
H	-2.215103	2.191423	-0.596261
H	-3.409557	-2.151750	0.504695
H	-6.100786	0.977685	0.057824
H	-4.417879	2.642747	-0.486410
H	-5.559194	-1.353715	0.526467
H	0.241586	1.393956	-0.381182
C	0.755819	2.760408	-0.484436
H	-0.110434	3.179581	-1.006012
C	1.971922	2.633107	-1.277286
C	3.207309	2.628624	-0.716376
C	3.431227	2.859895	0.760863
C	2.156670	3.189509	1.500432
C	0.941782	3.160438	0.911973
H	1.870528	2.492529	-2.353211
H	4.089642	2.510858	-1.345264
H	3.911479	1.973595	1.218982
H	2.248507	3.461466	2.550889
H	0.055630	3.406809	1.496041
H	4.172387	3.668182	0.903058
N	2.475094	-0.622917	-0.375670
N	1.347523	-3.031263	0.277049
C	3.598157	-1.307551	-0.315167
C	2.590626	-3.461735	0.267243
C	3.712782	-2.671626	-0.009016
H	2.575189	0.364838	-0.618589
H	0.613473	-3.698128	0.489542
H	4.696182	-3.126761	0.010107
H	4.522937	-0.760020	-0.523581
H	2.752446	-4.520372	0.492972

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Cu	0.570984	1.370380	-0.081326
Pd	-1.950486	-0.119113	-0.044636
O	0.043301	-0.417333	-0.345515
O	-1.222595	1.699352	0.162810
N	2.409404	0.965188	-0.353597
N	0.946356	3.195978	0.216931
C	3.423412	1.801628	-0.297739
C	2.112047	3.804441	0.210706
C	3.340423	3.177034	-0.031353
H	2.644685	-0.009226	-0.558687
H	0.117976	3.750827	0.405462
P	-2.534845	-2.338498	-0.345370
P	-3.906912	0.966093	0.385423
H	4.249275	3.767403	-0.013790
H	4.419484	1.383201	-0.475770
H	2.117567	4.881143	0.410080
H	-3.880187	-2.763206	-0.259395
H	-5.193184	0.379065	0.421551
H	-1.981141	-3.315225	0.509183
H	-4.188152	2.039186	-0.478494
H	-2.226640	-2.959698	-1.574072
H	-3.953193	1.646539	1.615353
H	0.560017	-1.444525	-0.405846
C	1.212795	-2.712645	-0.516071
H	0.481863	-3.281795	-1.099845
C	1.417330	-3.155916	0.871230
C	2.583756	-2.988940	1.526913
C	3.803887	-2.372076	0.880705
C	3.619451	-2.149010	-0.605464
C	2.437016	-2.358673	-1.234093
H	0.573564	-3.608225	1.394167
H	2.677672	-3.302558	2.565864
H	4.054318	-1.418076	1.383916
H	4.499097	-1.863595	-1.182961
H	2.370801	-2.206246	-2.311635
H	4.689681	-3.010082	1.055125

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Cu	-0.949537	-1.354926	-0.081779
Pt	1.691814	-0.008734	-0.033843
O	-0.292611	0.394388	-0.362714
O	0.824145	-1.784381	0.183730
N	-2.754103	-0.829205	-0.378788
N	-1.451798	-3.146248	0.238509
C	-3.823758	-1.593167	-0.320954
C	-2.656259	-3.673551	0.228175
C	-3.836638	-2.967231	-0.035988
H	-2.919028	0.158666	-0.593495
H	-0.664098	-3.752310	0.444074
P	2.393486	2.141675	-0.366601
P	3.642095	-1.033121	0.409254
H	-4.783766	-3.494025	-0.019252
H	-4.787771	-1.110371	-0.512117
H	-2.737966	-4.744259	0.442893
H	3.769153	2.464926	-0.332969
H	4.719410	-0.999136	-0.502575
H	1.941055	3.159857	0.499678
H	3.481984	-2.421051	0.560847
H	2.084283	2.767060	-1.592899
H	4.366406	-0.733354	1.583014
H	-0.702483	1.448010	-0.416892
C	-1.264627	2.796936	-0.515289
H	-0.500734	3.318339	-1.099873
C	-1.428756	3.228159	0.878966
C	-2.594096	3.104931	1.547553
C	-3.847887	2.551005	0.908500
C	-3.693706	2.348942	-0.584496
C	-2.508641	2.514741	-1.224434
H	-0.559192	3.635010	1.396840
H	-2.661069	3.408337	2.591529
H	-4.129210	1.598366	1.398143
H	-4.593630	2.122561	-1.156811
H	-2.462588	2.381645	-2.305545
H	-4.704139	3.221022	1.108588

Table S2. Dichloromethane solvation free energies for **1**-**6**.

Complex	ΔG_{solv} (Kcal/mol)
1	-14.2
2	-10.5
3	-10.9
4	-59.5
5	-50.9
6	-54.5

Table S3. Aqueous solvation free energies for **1**-**3** and **7**-**9**.

Complex	ΔG_{solv} (Kcal/mol)
1	-14.3
2	-9.4
3	-10.4
7	-53.0
8	-41.0
9	-41.8

(1) Aboelella, N. W.; York, J. T.; Reynolds, A. M.; Fujita, K.; Kinsinger, C. R.; Cramer, C. J.; Riordan, C. G.; Tolman, W. B., *Chem. Commun.* **2004**, 1716-1717.