Supplementary Material (ESI) for New Journal of Chemistry

Photo-Induced Self-Assembly of Pt(II)-Linked Rings and Cages via the Photolabilization of a Pt(II)−Pyridine Bond

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Contents;

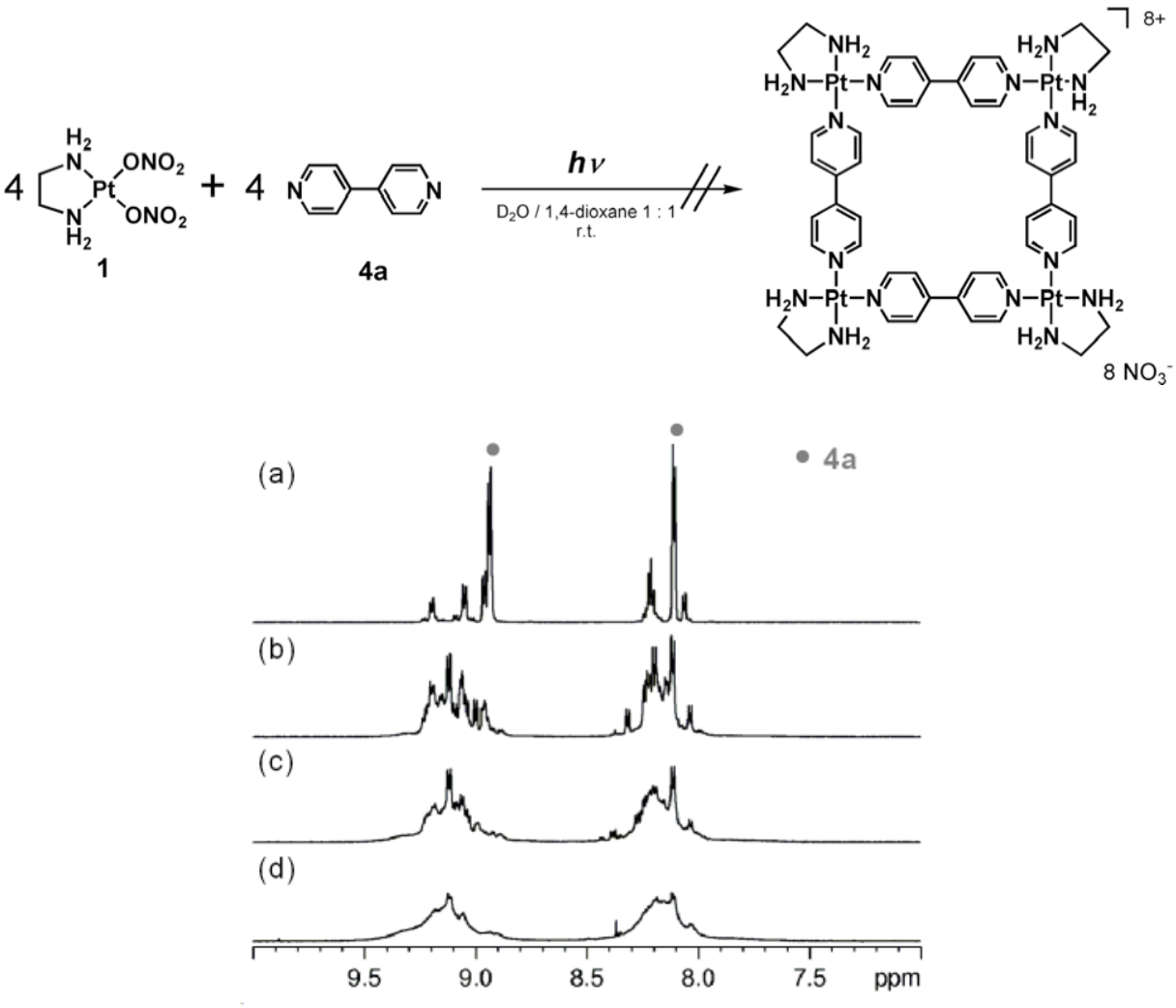

Figure S1. ^{1}H NMR observation of the self-assembly from ligand **4a** by UV irradiation (Aromatic region, 500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before irradiation, and after irradiation for (b) 1 h, (c) 3 h, and (d) 6 hours.

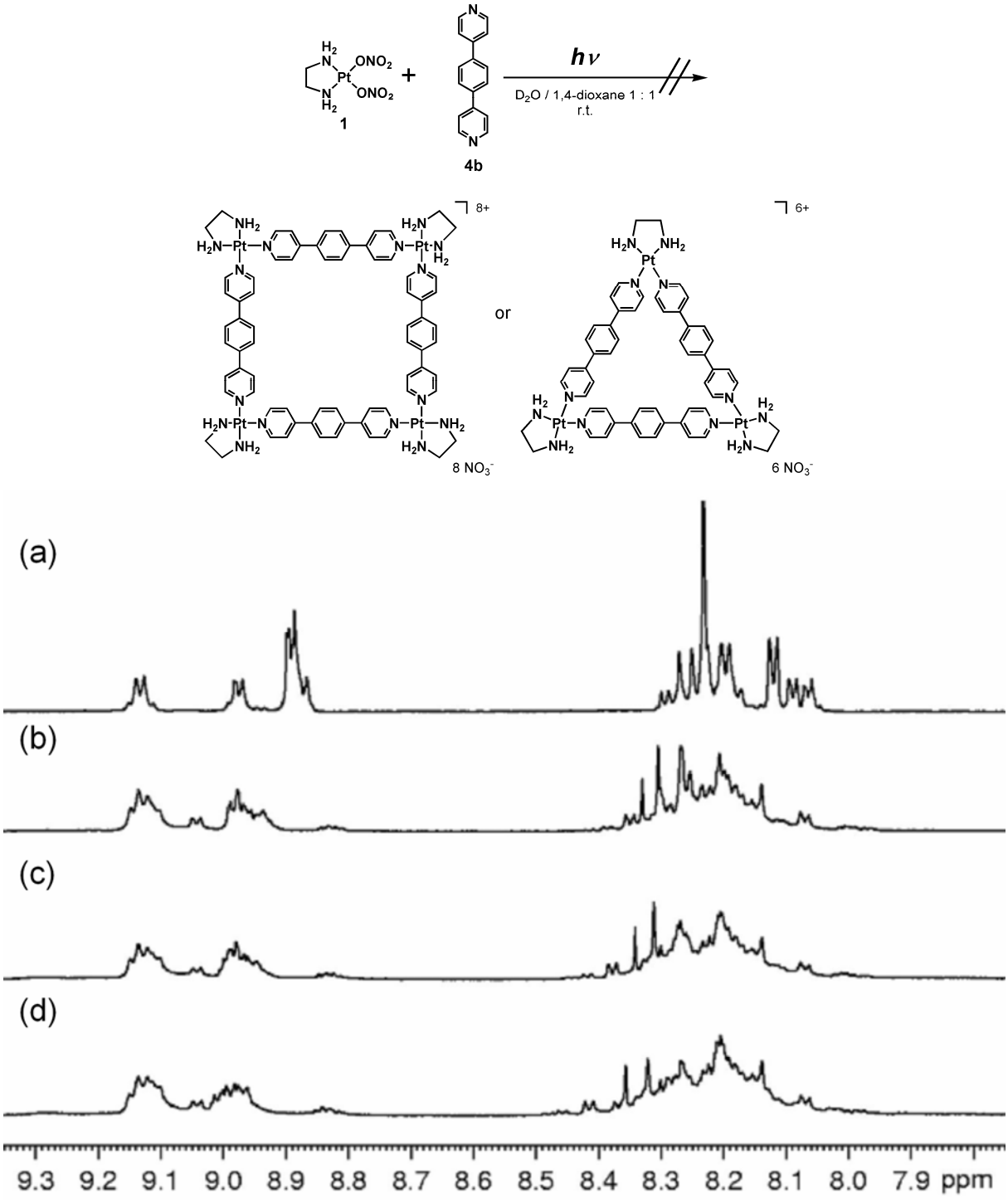

Figure S2. ^{1}H NMR observation of the self-assembly from ligand **4b** by UV irradiation (500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before irradiation, and after irradiation for (b) 15 min, (c) 60 min, and (d) 240 min.

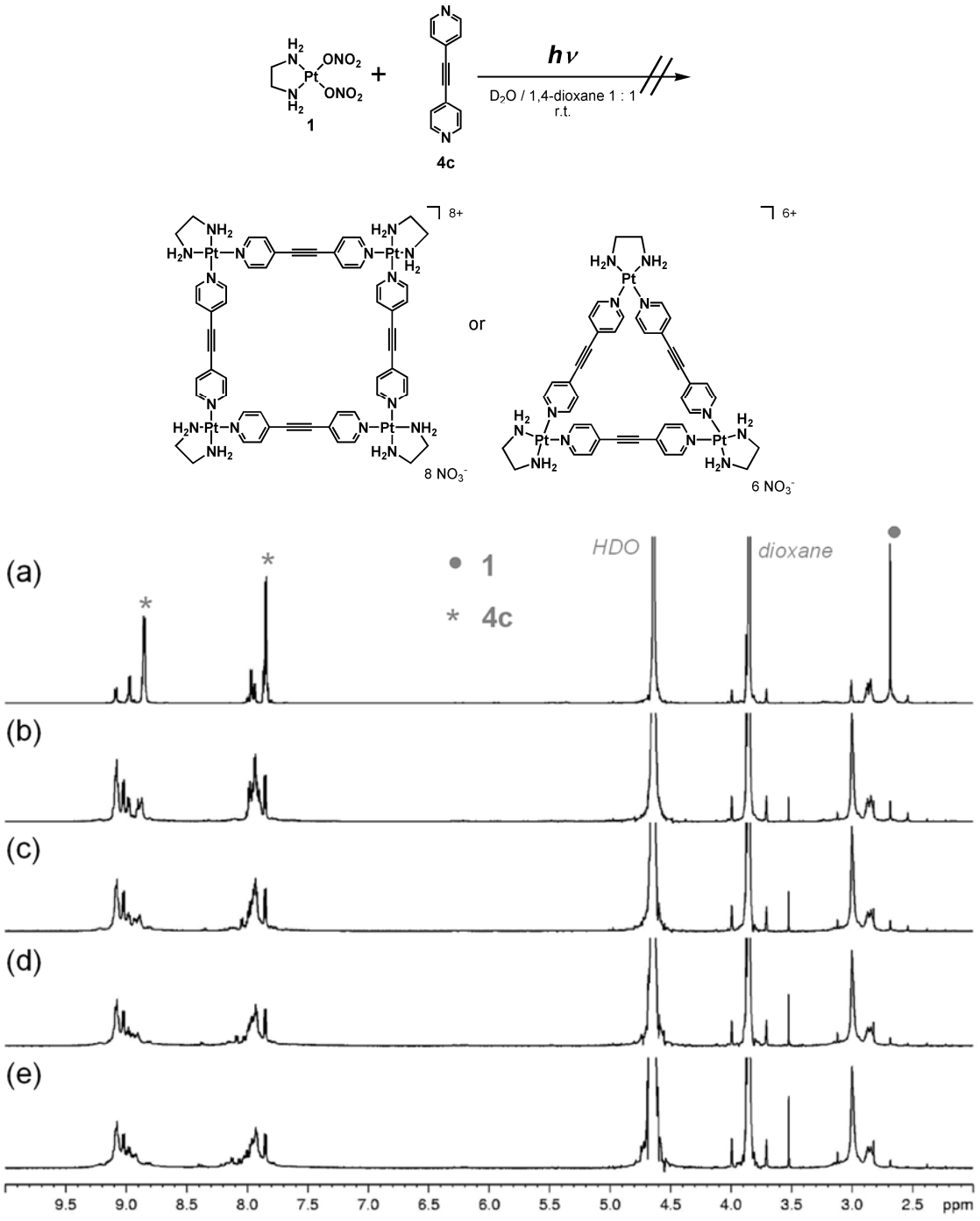

Figure S3. ^{1}H NMR observation of the self-assembly from ligand **4c** by UV irradiation (500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before irradiation, and after irradiation for (b) 30 min, (c) 60 min, (d) 90 min, and (e) 120 min.

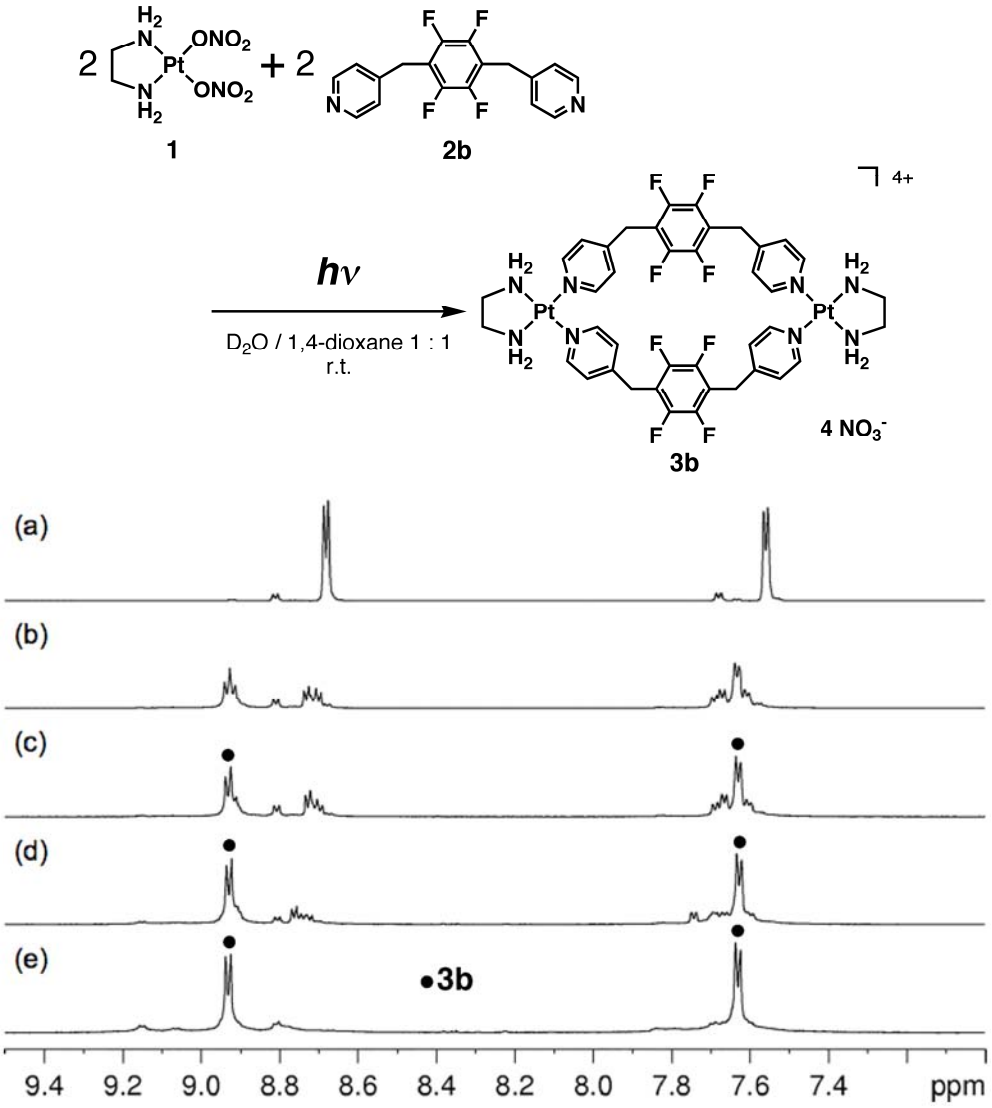

Figure S4. ^{1}H NMR observation of the self-assembly from ligand **2b** by UV irradiation (500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before irradiation, and after irradiation for (b) 15 min, (c) 30 min, (d) 60 min, and (e) 120 min.

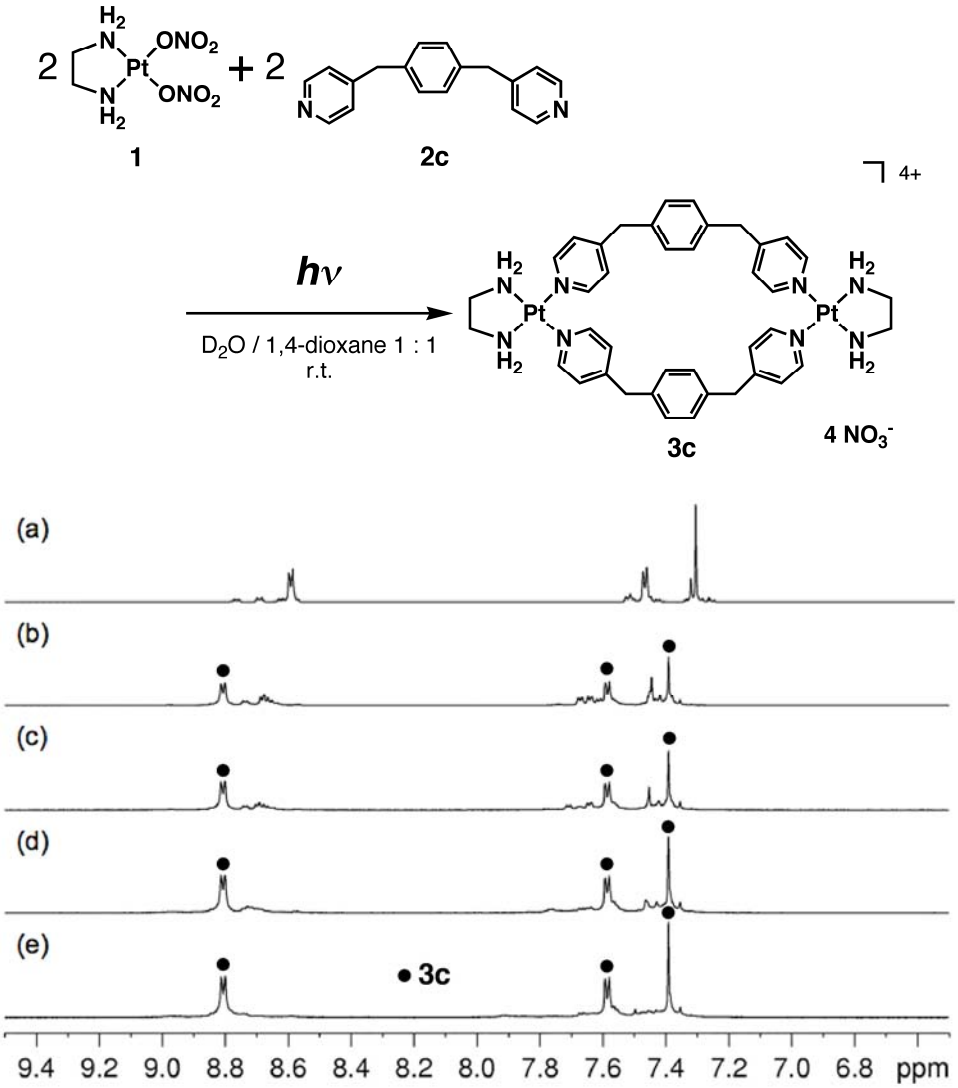

Figure S5. ^{1}H NMR observation of the self-assembly from ligand **2c** by UV irradiation (500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before irradiation, and after irradiation for (b) 15 min, (c) 30 min, (d) 60 min, and (e) 180 min.

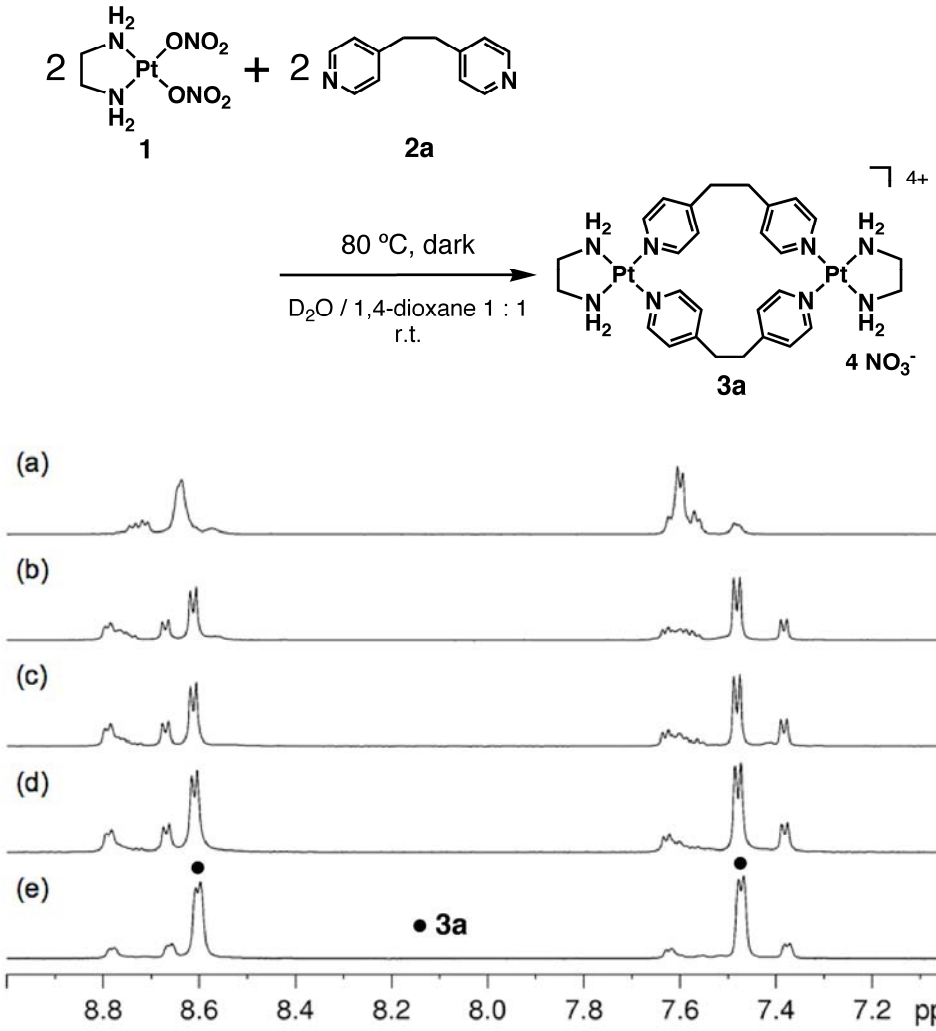

Figure S6. ^{1}H NMR observation of the self-assembly from ligand **2a** after heating at 80ºC without UV irradiation (500 MHz, D_2O/1,4-dioxane-d_8 1:1): (a) before heating, and after heating for (b) 4 h, (c) 1 d, (d) 8 d, and (e) 36 d.

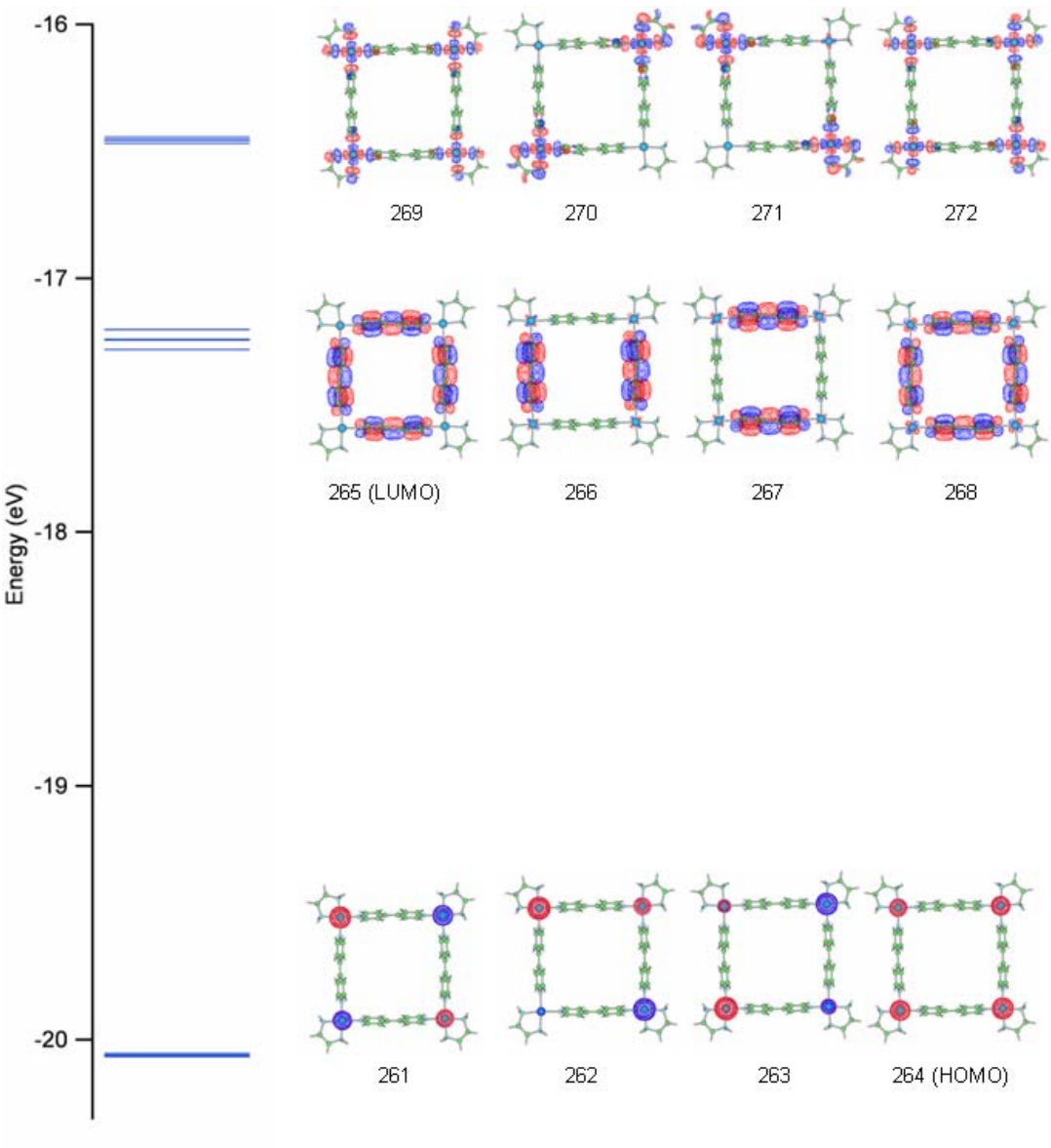

Figure S7. Frontier energy level scheme and some related molecular orbitals for $[(en)Pt(\mathbf{4a})]_4^{8+}$, as calculated using DFT.

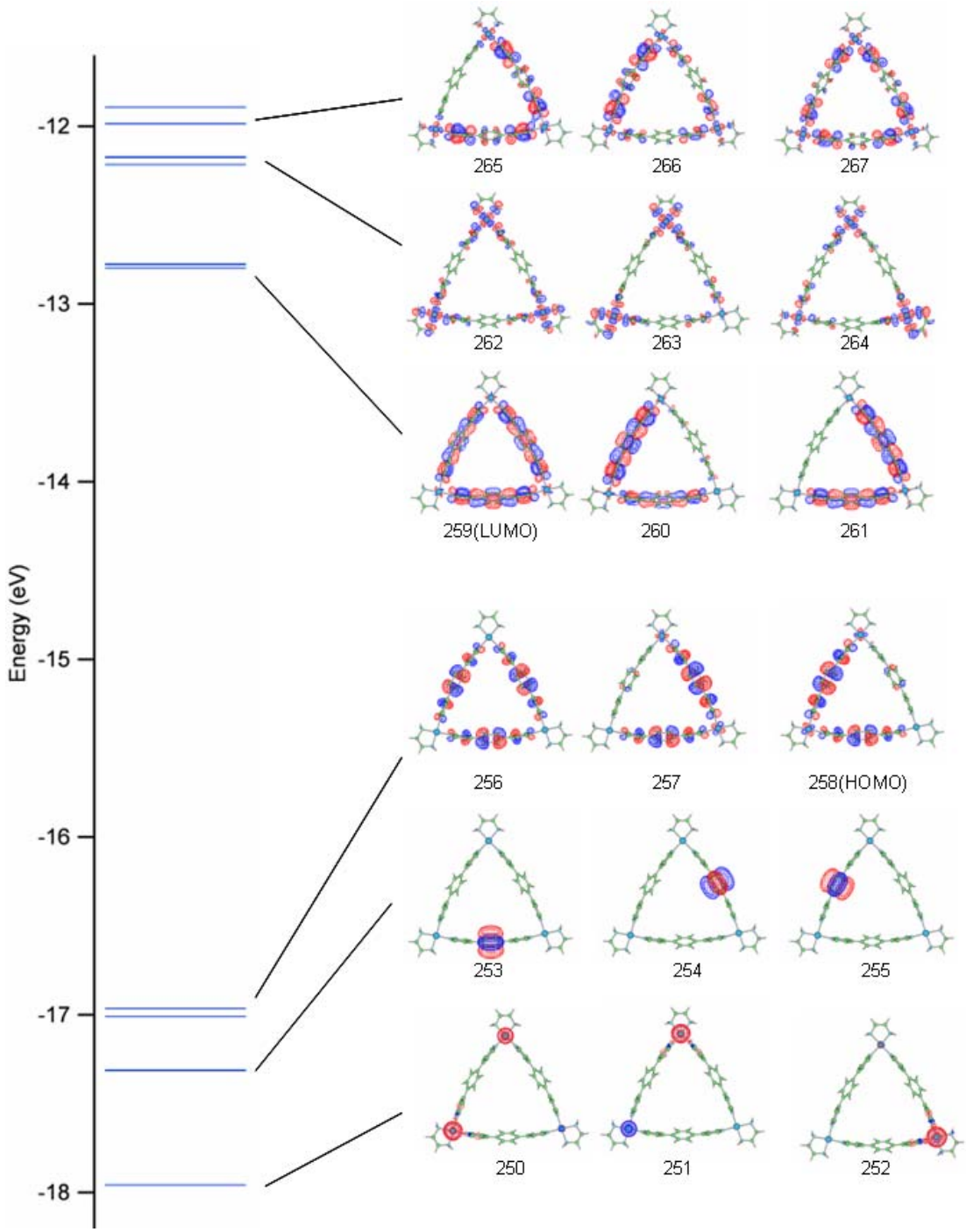

Figure S8. Frontier energy level scheme and some related molecular orbitals for $[(en)Pt(\mathbf{4b})]_3^{6+}$, as calculated using DFT.

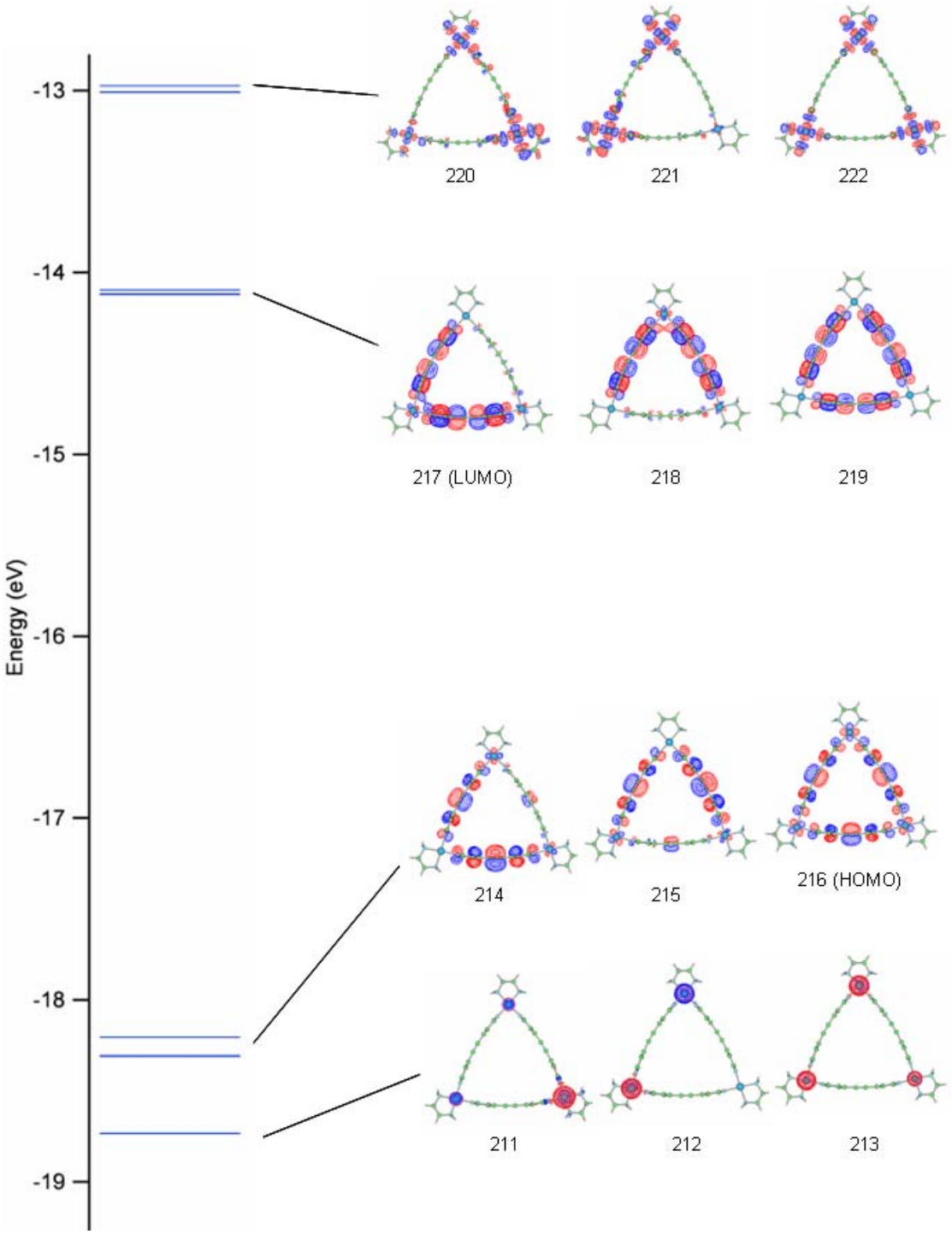

Figure S9. Frontier energy level scheme and some related molecular orbitals for $[(en)Pt(\mathbf{4c})]_3^{6+}$, as calculated using DFT.

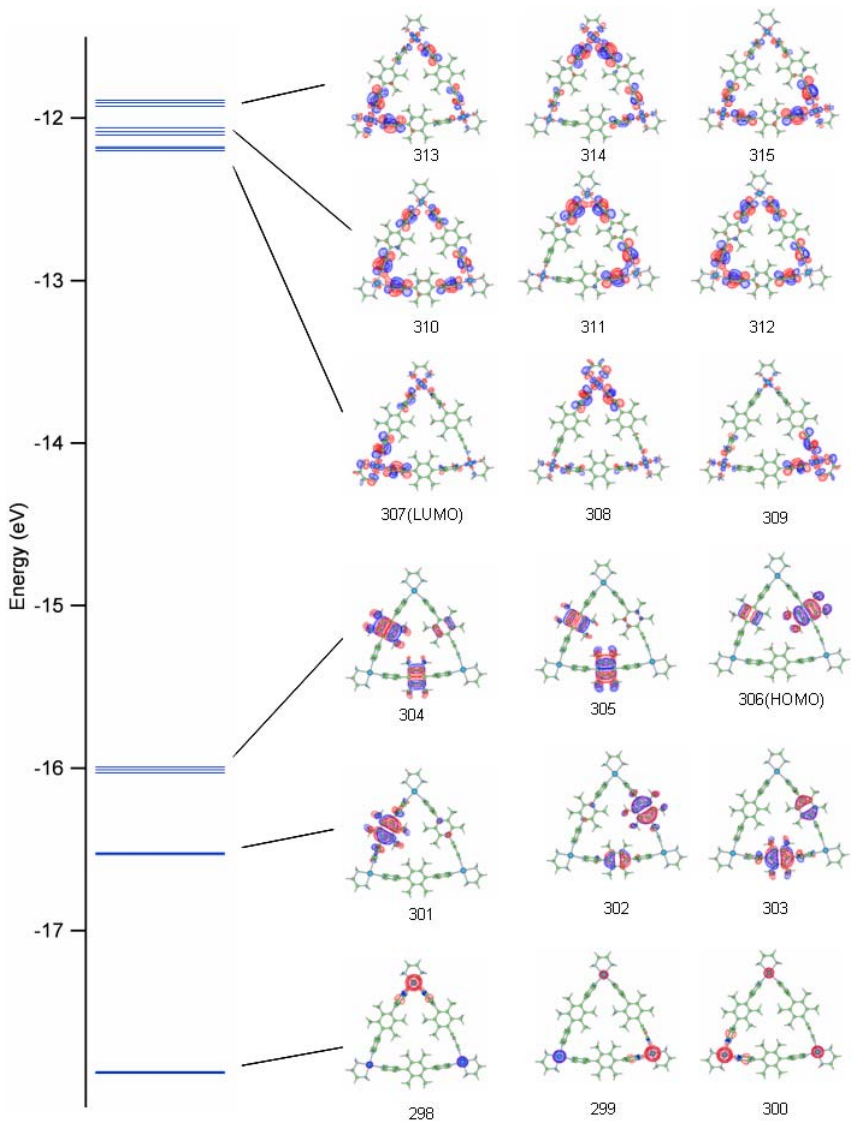

Figure S10. Frontier energy level scheme and some related molecular orbitals for $[(en)Pt(\mathbf{4d})]_3^{6+}$, as calculated using DFT.

Table S1. Cartesian Coordinates of $[(en)Pt(\mathbf{4a})]_4^{8+}$ optimized using the B3LYP level of the theory with the LANL2DZ basis set for Pt, and 6-31G* for the other atoms, respectively.

[(en)Pt(**4a**)]4 8+

Symmetry C1; singlet state; HF = −3216.0316045

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	-2.715133	6.660755	-1.983701
C	-2.912899	6.066984	-1.097768
N	-2.228562	6.394997	0.024664
C	-3.834670	5.024534	-1.137744
C	-4.086326	4.254504	0.012463
C	-2.480010	5.681081	1.146923
H	-4.361164	4.847938	-2.069168
C	-3.383343	4.622310	1.174174
H	-1.942479	5.971752	2.042193
C	-5.027494	3.089607	0.001360
H	-3.512142	4.089874	2.109812
C	-5.242156	2.325348	-1.160250
C	-5.725206	2.680430	1.151967
H	-4.749470	2.563316	-2.097752
C	-6.550702	1.558838	1.112886
C	-6.086255	1.218290	-1.132184
H	-5.663219	3.231898	2.083641
Pt	-0.861383	8.013833	0.026687
N	6.726057	-0.820363	-0.011777
N	-6.728337	0.821761	-0.009188
H	-6.257590	0.631000	-2.027572
H	-7.088053	1.241583	2.000281
N	0.338325	9.734091	-0.039652
C	6.079134	-1.213328	-1.133672
C	6.551833	-1.562338	1.108998
H	1.171415	9.681058	0.553987
H	0.689798	9.852274	-0.995903
C	-0.472205	10.955770	0.345096
H	6.248418	-0.623174	-2.027651
C	5.726512	-2.682675	1.146287
C	5.234077	-2.318900	-1.162666
H	7.092682	-1.247355	1.994891
C	-1.839903	10.817030	-0.292427
H	0.037586	11.863340	0.010785
H	-0.534263	10.978340	1.437573
Pt	-8.017461	-0.860716	-0.020401
N	-6.393048	-2.221763	-0.012823
C	5.023829	-3.087617	-0.003148
H	4.738857	-2.554738	-2.097876
H	5.666758	-3.238347	2.077146
N	-2.387406	9.453619	0.082864
H	-2.523916	11.600430	0.046057
H	-1.783272	10.858740	-1.383892
C	-6.052902	-2.909746	-1.130006
C	-5.690526	-2.469268	1.117124
C	4.082776	-4.251997	0.006861
Pt	0.860677	-8.014961	0.023356
H	-2.769363	9.495488	1.034316
H	-3.182587	9.232444	-0.521834
H	-6.636143	-2.715023	-2.023235
C	-4.631433	-3.372002	1.157701
C	-5.008937	-3.831592	-1.155429
H	-5.991099	-1.928058	2.006826
C	3.828884	-5.017496	-1.145080
C	3.381429	-4.624481	1.167388
N	0.813463	6.717100	0.014747
C	-4.250686	-4.079276	0.003162
H	-4.823253	-4.360508	-2.084312
H	-4.107967	-3.496723	2.099936
N	9.442606	2.399235	-0.033384
Pt	8.015718	0.861077	-0.023750
H	4.354538	-4.837882	-2.078346
C	2.477922	-5.682508	1.138493
C	2.907401	-6.060174	-1.107798
H	3.511396	-4.094323	2.105515
C	1.202978	6.079275	-1.113927

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	1.557546	6.532286	1.131471
C	-3.085586	-5.020016	0.005112
H	9.213280	3.156795	0.617350
H	9.480433	2.832983	-0.962320
C	10.812340	1.845891	0.306577
N	2.224368	-6.392563	0.013754
H	2.707391	-6.650043	-1.997094
H	1.939620	-5.976190	2.032705
C	2.679418	5.706758	1.158967
C	2.308310	5.234562	-1.152372
H	1.244704	7.065644	2.023137
H	0.610190	6.255547	-2.004094
C	-2.684827	-5.711816	1.162459
C	-2.313459	-5.240939	-1.149546
C	10.954010	0.510948	-0.398354
H	10.863130	1.738087	1.393395
H	11.588700	2.550357	-0.005447
H	3.236855	5.640800	2.088021
C	3.080554	5.014816	0.002663
H	2.540953	4.747206	-2.093281
H	-3.243393	-5.644132	2.090507
C	-1.208578	-6.085213	-1.110651
C	-1.564383	-6.538230	1.135751
H	-2.546072	-4.753456	-2.090646
N	9.745231	-0.327313	-0.034048
H	10.960240	0.625170	-1.486207
H	11.871560	-0.006502	-0.102005
N	-9.746505	0.328047	-0.033183
C	4.247493	4.076596	0.000704
N	-0.819571	-6.722227	0.019177
H	-1.252759	-7.071263	2.026808
H	-0.615784	-6.263513	-2.000270
H	9.677614	-1.121112	-0.679392
H	9.892512	-0.737068	0.894527
H	-9.679080	1.120673	-0.678730
H	-9.894107	0.737453	0.895154
C	-10.954710	-0.512612	-0.396793
C	5.005204	3.829736	-1.158260
C	4.629053	3.369906	1.154779
C	-10.814350	-1.845203	0.311777
H	-10.959140	-0.628986	-1.484289
H	-11.871920	0.005762	-0.102888
C	5.689092	2.467770	1.114055
C	6.050466	2.908998	-1.132467
H	4.105688	3.494277	2.097541
H	4.818386	4.359001	-2.087228
N	-9.443397	-2.399318	-0.022887
H	-10.866360	-1.734359	1.398341
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H	5.989728	1.927181	2.004031
N	6.391897	2.222420	-0.016276
H	6.634679	2.715655	-2.025839
H	-9.214837	-3.152666	0.632594
H	-9.480471	-2.839909	-0.949410
N	-0.330501	-9.742187	0.028575
H	-1.123592	-9.680425	-0.616366
H	-0.740124	-9.879685	0.958854
C	0.507854	-10.955140	-0.322624
C	1.840448	-10.809940	0.384182
H	0.624309	-10.970470	-1.409936
H	-0.012138	-11.868550	-0.020418
N	2.396659	-9.443193	0.035855
H	1.729748	-10.851090	1.471048
H	2.545482	-11.589270	0.080204
H	2.837285	-9.489172	-0.889385
H	3.150633	-9.209325	0.689490

Table S2. Cartesian Coordinates of $[(en)Pt(\mathbf{4b})]_3^{6+}$ optimized using the B3LYP level of the theory with the LANL2DZ basis set for Pt, and 6-31G* for the other atoms, respectively.

[(en)Pt(**4b**)]3 6+

Symmetry C1; singlet state; HF = −3106.667146

	Coordinates (Angstroms)		
Atom	X	Y	Z
Pt	−0.1786146	8.9085040	−0.0050050
N	−1.5883247	10.4689190	−0.0269650
N	1.1685843	10.5231290	0.0156340
N	1.3061553	7.4436930	0.0145170
N	−1.6033716	7.3851066	−0.0241150
C	−0.9154186	11.7742810	0.3278970
C	0.4452874	11.7992080	−0.3464710
C	1.7098614	6.8467693	−1.1324370
C	1.8363754	7.0028934	1.1807820
C	−2.1265147	6.9325323	−1.1891060
C	−1.9715617	6.7627144	1.1212940
H	−2.3694465	10.2993765	0.6124540
H	−2.0064256	10.5426840	−0.9599240
H	1.5796754	10.6167670	0.9499580
H	1.9582454	10.3825340	−0.6202880
C	2.6002665	5.7828794	−1.1424740
C	2.7312574	5.9446400	1.2375749
C	−2.9787307	5.8395243	−1.2466020
C	−2.8182597	5.6638374	1.1304330
H	−0.8215416	11.8085570	1.4168789
H	−1.5338186	12.6184260	0.0094230
H	1.0300233	12.6686610	−0.0325320
H	0.3503534	11.8236360	−1.4356240
H	1.2886194	7.2297290	−2.0550740
H	1.5257983	7.5182133	2.0829390
H	−1.8452417	7.4667993	−2.0898430
H	−1.5581176	7.1551642	2.0434470
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C	−3.3297656	5.1428275	−0.0736840
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H	3.1292834	5.6596313	2.2052980
H	−3.3741026	5.5469465	−2.2131160
H	−3.0428867	5.1971720	2.0831919
C	3.9786403	4.0619383	0.0926530
C	−4.1397950	3.8996224	−0.1050800
C	3.8953714	3.1641004	1.1727610
C	4.8460200	3.7415144	−0.9688440
C	−4.0389605	3.0170975	−1.1964290
C	−4.9768760	3.5340183	0.9661680
C	4.6147094	1.9739434	1.1718090
C	5.5672693	2.5502925	−0.9690200
C	−4.7113347	1.7996254	−1.1976041
C	−5.6503660	2.3152544	0.9648050
H	3.2277904	3.3681004	2.0040040
H	4.9849253	4.4347734	−1.7927910
H	−3.3930807	3.2551303	−2.0357130
H	−5.1299725	4.2125115	1.7998530
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C	−5.5131207	1.4135153	−0.1076240
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H	6.2460194	2.3532624	−1.7931200
H	−4.5680456	1.1274784	−2.0377260
H	−6.3069570	2.0822904	1.7975069
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C	−6.1337285	0.0655064	−0.0777160
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C	6.5175223	−0.3613276	1.2324450
C	−6.3033630	−0.6448596	1.1262420
C	−6.5334260	−0.6035476	−1.2511901
C	6.8829565	−1.6571406	−1.1459190
C	7.0385375	−1.6454417	1.1703700
C	−6.7806050	−1.9472547	1.1164500
C	−7.0021477	−1.9080156	−1.1943720
H	6.0875554	0.0661374	−2.1047310
H	6.4340105	0.1116204	2.2047250
H	−6.0301547	−0.2057316	2.0793810
H	−6.4946184	−0.1135266	−2.2178560
N	7.2037480	−2.3058636	−0.0009950
N	−7.1073976	−2.5916877	−0.0292810
H	7.0442524	−2.1960256	−2.0727630
H	7.3317223	−2.1716866	2.0719700
H	−6.8934455	−2.5063405	2.0383940
H	−7.2999250	−2.4318907	−2.0959120
Pt	7.8086870	−4.3015485	−0.0314330
Pt	−7.6296697	−4.6110125	−0.0035730
N	8.5334010	−6.2758417	−0.0503260
N	9.8638400	−3.8610446	−0.0822530
N	5.7970624	−4.8523655	0.0007040
N	−5.5966744	−5.0773535	0.0196320
N	−9.7021310	−4.2574105	−0.0372450
N	−8.2709980	−6.6132965	0.0310590
C	9.9958230	−6.2833977	−0.4298300
C	10.6633700	−5.0995345	0.2481150
C	5.0760984	−4.9125120	−1.1445290
C	5.1513824	−5.0797877	1.1699000
C	−4.9407897	−5.3038260	1.1834440
C	−4.8755574	−5.0825458	−1.1269860
C	−10.4454270	−5.5216227	0.3263950
C	−9.7348750	−6.6900754	−0.3344910
H	8.0091050	−6.8808610	−0.6880740
H	8.4193900	−6.6913950	0.8797010
H	10.1168950	−3.5303047	−1.0189750
H	10.1226820	−3.1035666	0.5557260
H	−9.9833360	−3.9543805	−0.9751970
H	−9.9811850	−3.5000696	0.5923660
H	−7.7270910	−7.2108965	−0.5973170
H	−8.1327490	−7.0018477	0.9694080
C	3.7090554	−5.1477256	−1.1509380
C	3.7871363	−5.3243084	1.2299010
C	−3.5675967	−5.4932265	1.2380760
C	−3.5002346	−5.2636185	−1.1389580
H	10.0515670	−6.2029867	−1.5189620
H	10.4601550	−7.2274010	−0.1304440
H	11.6989290	−4.9820485	−0.0839230
H	10.6616450	−5.2099996	1.3360690
H	5.6174426	−4.7506127	−2.0698900
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C	3.0080783	−5.3332660	0.0562110
C	−2.7911577	−5.4466860	0.0637420
H	3.1933393	−5.1471214	−2.1048310
H	3.3432283	−5.5188210	2.2000110
H	−3.1140077	−5.6891274	2.2034800
H	−2.9853616	−5.2226534	−2.0924660
C	1.5304774	−5.4692316	0.0885060
C	−1.3092836	−5.5247436	0.0919880
C	−0.5760596	−6.0707874	−0.9785700
C	0.8161314	−6.0441966	−0.9798700
C	0.7968184	−4.9640536	1.1778200
C	−0.5936146	−4.9916835	1.1798459
H	−1.0887076	−6.5465736	−1.8090351
H	1.3442384	−6.5009785	−1.8112250
H	1.3084334	−4.5012090	2.0157670
H	−1.1214746	−4.5500546	2.0192199

Table S3. Cartesian Coordinates of $[(en)Pt(\mathbf{4c})]_3^{6+}$ optimized using the B3LYP level of the theory with the LANL2DZ basis set for Pt, and 6-31G* for the other atoms, respectively.

[(en)Pt(**4c**)]3 6+

Symmetry C1; singlet state; HF = −2641.8701732

	Coordinates (Angstroms)		
Atom	X	Y	Z
Pt	2.0969100	7.6203480	−0.0022996
N	1.1824139	9.5108940	−0.0256656
N	3.8385570	8.7935870	0.0204234
N	3.1139948	5.7889290	0.0017574
N	0.2945119	6.5530653	−0.0061716
C	2.1912120	10.5795950	0.3327743
C	3.5048220	10.2243310	−0.3396117
H	0.3794639	9.5720630	0.6066524
H	0.8094599	9.6962240	−0.9627376
H	4.2539850	8.7669000	0.9575884
H	4.5633750	8.4417590	−0.6113936
C	3.4101630	5.1613083	−1.1623276
C	3.4142140	5.1625590	1.1653154
C	−0.2817221	6.1657170	−1.1698997
C	−0.2806281	6.1644893	1.1578404
H	2.2869978	10.5878950	1.4220704
H	1.8303789	11.5611250	0.0119244
H	4.3108697	10.8911840	−0.0200126
H	3.4256170	10.2782540	−1.4289297
C	3.9583240	3.8866212	−1.2025876
H	3.1893878	5.6994360	−2.0773716
H	3.1967678	5.7014780	2.0806124
C	3.9623039	3.8877770	1.2049273
C	−1.4034451	5.3490033	−1.2096926
H	0.1811889	6.5171650	−2.0851545
H	0.1835239	6.5149150	2.0729473
C	−1.4026201	5.3481130	1.1978763
H	4.1686960	3.4297931	−2.1631386
H	4.1758447	3.4318480	2.1652102
C	4.2190470	3.1999412	0.0010574
H	−1.8188851	5.0648320	−2.1700356
H	−1.8173041	5.0632000	2.1583273
C	−1.9770061	4.8906293	−0.0058666
C	−3.0578170	3.9586360	−0.0059906
C	4.6697390	1.8457441	0.0006534
C	−3.9268732	3.1064710	−0.0065426
C	4.9778900	0.6682162	−0.0003626
C	5.2483110	−0.7331588	−0.0012636
C	−4.8786740	2.0430400	−0.0076756
C	5.3634550	−1.4575459	−1.2054896
C	5.3558160	−1.4602609	1.2020143
C	−5.3573240	1.4848821	1.1954243
C	−5.3365100	1.4702941	−1.2120327
H	5.3282620	−0.9546258	−2.1654077
C	5.5092650	−2.8375030	−1.1667967
C	5.5015460	−2.8401258	1.1609683
H	5.3146367	−0.9595258	2.1628313
H	−5.0749960	1.9014982	2.1558073
C	−6.1909270	0.3756222	1.1548394
C	−6.1706530	0.3614812	−1.1727986
H	−5.0375140	1.8754241	−2.1722746
H	5.5848780	−3.4130460	−2.0825326
N	5.5520460	−3.5315409	−0.0036056
H	5.5710540	−3.4182530	2.0756145
H	−6.5574930	−0.0767299	2.0695574
N	−6.5767493	−0.2017579	−0.0090596
H	−6.5208783	−0.1015478	−2.0884457
Pt	5.5573310	−5.6264770	−0.0010786
Pt	−7.6569370	−1.9964489	−0.0029106
N	5.6791820	−7.7229137	0.0191624
N	7.6498620	−5.8030868	−0.0254206
N	3.4631520	−5.5720300	0.0074244
N	−5.8312670	−3.0235120	0.0091334
N	−9.5433340	−1.0739789	−0.0331716
N	−8.8384010	−3.7326320	0.0229624
C	7.0817280	−8.1655300	−0.3350636
C	8.0545160	−7.2143390	0.3381434
H	5.0095660	−8.1658730	−0.6162676
H	5.4398500	−8.0679455	0.9547384
H	7.9984650	−5.5806127	−0.9637907
H	8.1130360	−5.1409187	0.6033583
C	2.7683640	−5.5183277	−1.1549187
C	2.7743490	−5.5078950	1.1726583
C	−5.2007560	−3.3070880	1.1745694
C	−5.2125130	−3.3461440	−1.1526647
C	−10.6159190	−2.0749250	0.3341454
C	−10.2693760	−3.3939087	−0.3326117
H	−9.7269650	−0.7093608	−0.9738817
H	−9.6017270	−0.2643758	0.5909123
H	−8.4913910	−4.4589310	−0.6098446
H	−8.8100010	−4.1482697	0.9600124
H	7.1724240	−8.1275410	−1.4241797
H	7.2437787	−9.1980730	−0.0123696
H	9.0840240	−7.4047437	0.0212034
H	8.0089520	−7.2983070	1.4274783
C	1.3909400	−5.3504057	−1.1921266
H	3.3417910	−5.6039740	−2.0711136
H	3.3522530	−5.5856676	2.0866764
C	1.3971989	−5.3392520	1.2154204
C	−3.9304142	−3.8649578	1.2173984
H	−5.7329183	−3.0684779	2.0885015
H	−5.7539500	−3.1378120	−2.0686536
C	−3.9425370	−3.9053378	−1.1897876
H	−11.5966130	−1.7108709	0.0142814
H	−10.6216070	−2.1653538	1.4239163
H	−10.3279140	−3.3201760	−1.4221036
H	−10.9384570	−4.1952750	−0.0059666
H	0.8874569	−5.3082037	−2.1514647
H	0.8986079	−5.2883520	2.1768863
C	0.6699529	−5.2231936	0.0129524
H	−3.4710140	−4.0648460	2.1789544
H	−3.4928440	−4.1371160	−2.1487827
C	−3.2514892	−4.1496787	0.0147704
C	−1.9016631	−4.6131296	0.0157044
C	−0.7276801	−4.9344000	0.0149704

Table S4. Cartesian Coordinates of $[(en)Pt(\mathbf{4d})]_3^{6+}$ optimized using the B3LYP level of the theory with the LANL2DZ basis set for Pt, and 6-31G* for the other atoms, respectively.

[(en)Pt(**4d**)]3 6+

Symmetry C1; singlet state; HF = −3578.4186019

	Coordinates (Angstroms)		
Atom	X	Y	Z
Pt	-8.2396950	-3.3979032	0.1311935
N	-10.2400810	-2.7746980	0.3228568
N	-9.1507810	-5.2900070	0.0081891
N	-6.2954693	-4.1293116	-0.0662269
N	-7.4390720	-1.4761294	0.2617317
C	-11.1656760	-3.8980765	-0.0807654
C	-10.5897130	-5.1960690	0.4585105
C	-5.4903990	-4.2500553	1.0161865
C	-5.7752490	-4.4157357	-1.2838342
C	-7.1851230	-0.9071703	1.4644437
C	-7.0637230	-0.8080456	-0.8547926
H	-10.4461450	-1.9413983	-0.2346390
H	-10.4281225	-2.5100782	1.2950877
H	-9.1174620	-5.6268044	-0.9591758
H	-8.6606310	-5.9956740	0.5643442
C	-4.1520150	-4.6057890	0.9076765
C	-4.4450283	-4.7796946	-1.4554614
C	-6.5071950	0.2998510	1.5851163
C	-6.3812260	0.4009853	-0.7982606
H	-11.2131810	-3.9073195	-1.1732976
H	-12.1730310	-3.7180002	0.3055502
H	-11.1564030	-6.0619836	0.1043428
H	-10.5920230	-5.2078495	1.5520431
H	-5.9377830	-4.0409690	1.9813997
H	-6.4458520	-4.3330603	-2.1322505
H	-7.5207353	-1.4505218	2.3410870
H	-7.3040524	-1.2734979	-1.8041710
C	-3.5776472	-4.8513727	-0.3516244
C	-6.0470320	0.9729299	0.4410905
H	-3.5534666	-4.6695000	1.8103979
H	-4.0855000	-4.9878473	-2.4579592
H	-6.3147830	0.6954821	2.5770915
H	-6.0861583	0.8793388	-1.7264202
C	-2.1028268	-5.1030474	-0.5006598
C	-5.1615796	2.1866890	0.5300995
C	-1.2885919	-4.0560300	-0.9866050
C	-1.5462844	-6.3444376	-0.1292000
C	-3.7698598	1.9787127	0.6407876
C	-5.7042365	3.4856346	0.4865156
C	0.1049037	-4.2457695	-1.0780208
C	-1.8585548	-2.7110097	-1.3896161
C	-2.4091399	-7.4961010	0.3373097
C	-0.1477495	-6.5343876	-0.2194945
C	-2.9066315	3.0894406	0.6915648
C	-3.1650462	0.5904799	0.6916620
C	-7.1958340	3.7172267	0.3932570
C	-4.8366380	4.6022153	0.5466945
C	0.9572159	-3.0905020	-1.5637385
C	0.4318829	-7.8799200	0.1574178
C	0.6661757	-5.4797650	-0.6809245
C	-1.4146953	2.8390648	0.7735542
C	-5.4306170	5.9927735	0.5273023
C	-3.4470692	4.3925586	0.6434532
H	-1.3575802	-1.8921100	-0.8595576
H	-2.9249806	-2.6238230	-1.1810961
H	-1.7191654	-2.5233932	-2.4618661
H	-2.1373882	-7.8227463	1.3481114
H	-2.2866620	-8.3685300	-0.3153075
H	-3.4717920	-7.2487626	0.3448557
H	-2.5545030	0.4552254	1.5925941

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	-3.9182696	-0.1979020	0.6921652
H	-2.5065866	0.4105845	-0.1682498
H	-7.5718274	4.2438526	1.2791812
H	-7.7577844	2.7855394	0.3054063
H	-7.4548836	4.3382654	-0.4715742
C	2.1615555	-5.6315450	-0.7287844
C	-2.4893749	5.5523000	0.6831443
H	0.6488349	-2.7580996	-2.5619192
H	2.0168657	-3.3404070	-1.6189502
H	0.8644164	-2.2213930	-0.8992178
H	-0.0031189	-8.6812720	-0.4511440
H	0.2201288	-8.1328650	1.2032577
H	1.5134702	-7.9242835	0.0199363
H	-0.8296067	3.7578385	0.7248015
H	-1.1449015	2.3297670	1.7073348
H	-1.0765423	2.1960568	-0.0485224
H	-6.1027484	6.1468360	1.3804070
H	-6.0282288	6.1643558	-0.3751397
H	-4.6687427	6.7733740	0.5681271
C	2.9439201	-5.5408797	0.4355175
C	2.8595912	-5.8006234	-1.9368424
C	-2.0620656	6.1977640	-0.4894674
C	-1.9063089	5.9901714	1.8847917
C	4.3307576	-5.5463705	0.3558549
C	4.2491720	-5.7955613	-1.9532150
C	-1.0592431	7.1580010	-0.4383205
C	-0.9050764	6.9538736	1.8716528
H	2.4763690	-5.4412520	1.4095283
H	2.3257760	-5.9147334	-2.8747175
H	-2.4891530	5.9376564	-1.4525368
H	-2.2089062	5.5631094	2.8352947
N	4.9849815	-5.6435194	-0.8259702
N	-0.4608704	7.5167670	0.7225947
H	4.9441915	-5.4549217	1.2450587
H	4.7976860	-5.8970027	-2.8834174
H	-0.7041791	7.6446395	-1.3400974
H	-0.4276280	7.2785800	2.7896183
Pt	7.0561400	-5.4119340	-0.9175187
Pt	1.1933990	8.7877530	0.7281615
N	9.1535560	-5.2922590	-1.0267755
N	7.4570840	-7.4645123	-1.1471757
N	6.7694270	-3.3581808	-0.6905044
N	2.4166408	7.1064340	0.5471050
N	0.0598503	10.5510530	0.8925321
N	2.7859814	10.1612970	0.7543020
C	9.7137490	-6.5953480	-1.5460334
C	8.9257790	-7.7289740	-0.9124754
C	6.9292035	-2.7584624	0.5138747
C	6.3199677	-2.6069953	-1.7235962
C	2.5815856	6.5025983	-0.6539289
C	2.9956565	6.5381210	1.6320627
C	0.9552735	11.7043070	1.2791830
C	2.2628524	11.5589140	0.5198000
H	9.5382630	-5.1030800	-0.0958789
H	9.4701160	-4.5200267	-1.6193540
H	6.8978767	-8.0443920	-0.5157616
H	7.2041063	-7.7626576	-2.0944520
H	-0.7048467	10.4673770	1.5676973
H	-0.3873216	10.7521340	-0.0076003
H	3.2577400	10.1220880	1.6633685

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	3.5051239	9.9416330	0.0599608
C	6.5975070	-1.4263604	0.7288383
C	5.9684990	-1.2719228	-1.5696626
C	3.2753773	5.3074846	-0.7934153
C	3.7044902	5.3451815	1.5550236
H	10.7795240	-6.6711210	-1.3119689
H	9.6004070	-6.5902880	-2.6336780
H	9.0826630	-7.7663436	0.1691927
H	9.2096000	-8.6973970	-1.3342515
H	7.3140090	-3.3754260	1.3186738
H	6.2284930	-3.1042087	-2.6826527
H	2.1321850	6.9923920	-1.5104930
H	2.8681288	7.0527220	2.5781390
H	1.1140193	11.6484610	2.3597882
H	0.4669263	12.6564900	1.0528703
H	2.9978096	12.2998270	0.8476141
H	2.1143274	11.6768050	-0.5571839
C	6.0640760	-0.6486737	-0.3135198
C	3.8349843	4.6712914	0.3282193
H	6.7341495	-1.0064853	1.7201208
H	5.5943900	-0.7272356	-2.4302344
H	3.3597083	4.8641040	-1.7800826
H	4.1378655	4.9353130	2.4615147
C	5.5456090	0.7456184	-0.0944954
C	4.4698610	3.3128557	0.2167608
C	5.7300300	3.1583545	-0.3976173
C	6.2728560	1.8620225	-0.5552903
C	4.2978845	0.9036135	0.5485812
C	3.7566433	2.1952527	0.7049300
C	6.5374804	4.3471146	-0.8708381
C	7.6373825	1.7155409	-1.1922092
C	3.4916122	-0.2775321	1.0501564
C	2.4003017	2.3265650	1.3672469
H	6.0377720	5.2979593	-0.6800389
H	6.7472490	4.2912955	-1.9456694
H	7.5098386	4.3880440	-0.3661149
H	7.6536850	2.1201030	-2.2111820
H	7.9678330	0.6769872	-1.2440641
H	8.3972060	2.2672575	-0.6262559
H	3.2976632	-0.1991622	2.1266440
H	3.9882200	-1.2325777	0.8792262
H	2.5123553	-0.3295134	0.5568533
H	2.4332275	1.9947878	2.4128300
H	1.6512606	1.7041028	0.8632985
H	2.0237140	3.3494017	1.3632644

Table S5. Cartesian Coordinates of **4b** optimized using the B3LYP level of the theory with the 6-31G* for all atoms.

4b

Symmetry C1; singlet state; HF = − 726.4372133

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.1743910	0.1481449	-5.0228285
C	-1.2165716	0.1566538	-3.6299064
N	-0.0524651	-0.0020915	-5.7382663
H	-2.0921984	0.2750116	-5.5950679
C	-0.0266023	-0.0010431	-2.9030029
C	1.0823882	-0.1518052	-5.0432744
H	-2.1622299	0.3106834	-3.1189785
C	1.1499503	-0.1592957	-3.6514002
C	-0.0130335	-0.0004901	-1.4203837
H	1.9895454	-0.2791650	-5.6321320
C	-1.0694424	-0.5634821	-0.6854528
C	1.0566626	0.5630200	-0.7053350
H	2.1047343	-0.3129866	-3.1576264
C	-1.0567061	-0.5629792	0.7053775
C	1.0693937	0.5635285	0.6854888
H	-1.8944071	-1.0374440	-1.2095500
H	1.8719029	1.0365635	-1.2448059
C	0.0129878	0.0005255	1.4203972
H	-1.8719332	-1.0365582	1.2448440
H	1.8943572	1.0374863	1.2096027
C	0.0265873	0.0010594	2.9030156
C	-1.1498966	0.1597569	3.6514123
C	1.2165258	-0.1571197	3.6298605
C	-1.0823072	0.1521295	5.0432890
C	1.1743944	-0.1485320	5.0227798
H	-2.1046171	0.3138234	3.1576330
H	2.1620875	-0.3115568	3.1188707
N	0.0525164	0.0020530	5.7382423
H	-1.9893934	0.2798851	5.6321778
H	2.0921565	-0.2759026	5.5949808

Table S6. Cartesian Coordinates of **4d** optimized using the B3LYP level of the theory with the 6-31G* for all atoms.

4d

Symmetry C1; singlet state; HF = −883.6884232

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.2451588	0.0332432	-5.0037712
C	-1.2701504	0.0303420	-3.6087716
N	-0.1214142	0.0156910	-5.7317585
H	-2.1779155	0.0506103	-5.5659624
C	-0.0613786	0.0078908	-2.9006988
C	1.0321802	-0.0057340	-5.0521710
H	-2.2180790	0.0453532	-3.0783382
C	1.1162892	-0.0104938	-3.6594892
C	-0.0296343	0.0037801	-1.4009720
H	1.9402624	-0.0198772	-5.6534875
C	0.0062935	1.2261301	-0.7014484
C	-0.0361950	-1.2223670	-0.7072102
H	2.0858510	-0.0282913	-3.1698087
C	0.0359319	1.2223003	0.7072175
C	-0.0065269	-1.2261973	0.7014505
C	-0.0743851	-2.5455411	-1.4425078
C	0.0139444	2.5532535	-1.4305487
C	0.0294349	-0.0038419	1.4009761
C	-0.0139871	-2.5533490	1.4305061
C	0.0744483	2.5454437	1.4425491
H	-0.9580438	-3.1331246	-1.1618907
H	0.7991922	-3.1635967	-1.1981285
H	-0.0945095	-2.4169911	-2.5249879
H	-0.8493820	3.1693463	-1.1477664
H	-0.0096739	2.4305091	-2.5136352
H	0.9079013	3.1399781	-1.1826991
C	0.0613236	-0.0079062	2.9006997
H	0.8496516	-3.1691401	1.1479839
H	-0.9076516	-3.1403661	1.1823329
H	0.0092236	-2.4306435	2.5136031
H	0.0926190	2.4168825	2.5250652
H	-0.7979343	3.1645694	1.1967117
H	0.9593222	3.1319324	1.1633939
C	1.2701544	-0.0304939	3.6086548
C	-1.1162732	0.0107340	3.6596061
C	1.2452961	-0.0333026	5.0036609
C	-1.0320327	0.0060004	5.0522759
H	2.2180355	-0.0456847	3.0781417
H	-2.0858741	0.0286936	3.1700086
N	0.1216289	-0.0155573	5.7317548
H	2.1781067	-0.0507954	5.5657594
H	-1.9400510	0.0203527	5.6536830

Table S7. Crystal data and structure refinement for **5**·$(H_2O)_m$.

Identification code	PtTriangle5	
Empirical formula	C66 H123 N18 O37.50 Pt3	
Formula weight	2354.09	
Temperature	80(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.8836(18) Å	α= 92.901(2)°.
	b = 18.679(3) Å	β= 94.205(2)°.
	c = 19.283(3) Å	γ = 100.971(2)°.
Volume	4885.4(11) $Å^3$	
Z	2	
Density (calculated)	1.600 Mg/m^3	
Absorption coefficient	4.372 mm^{-1}	
F(000)	2358	
Crystal size	0.16 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.91 to 28.87°.	
Index ranges	-18<=h<=18, -24<=k<=25, -25<=l<=25	
Reflections collected	56156	
Independent reflections	22988 [R(int) = 0.0229]	
Completeness to theta = 28.87°	89.5 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.6689 and 0.5413	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	22988 / 780 / 1391	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.1068	
R indices (all data)	R1 = 0.0486, wR2 = 0.1157	
Largest diff. peak and hole	3.048 and -2.009 $e.Å^{-3}$	

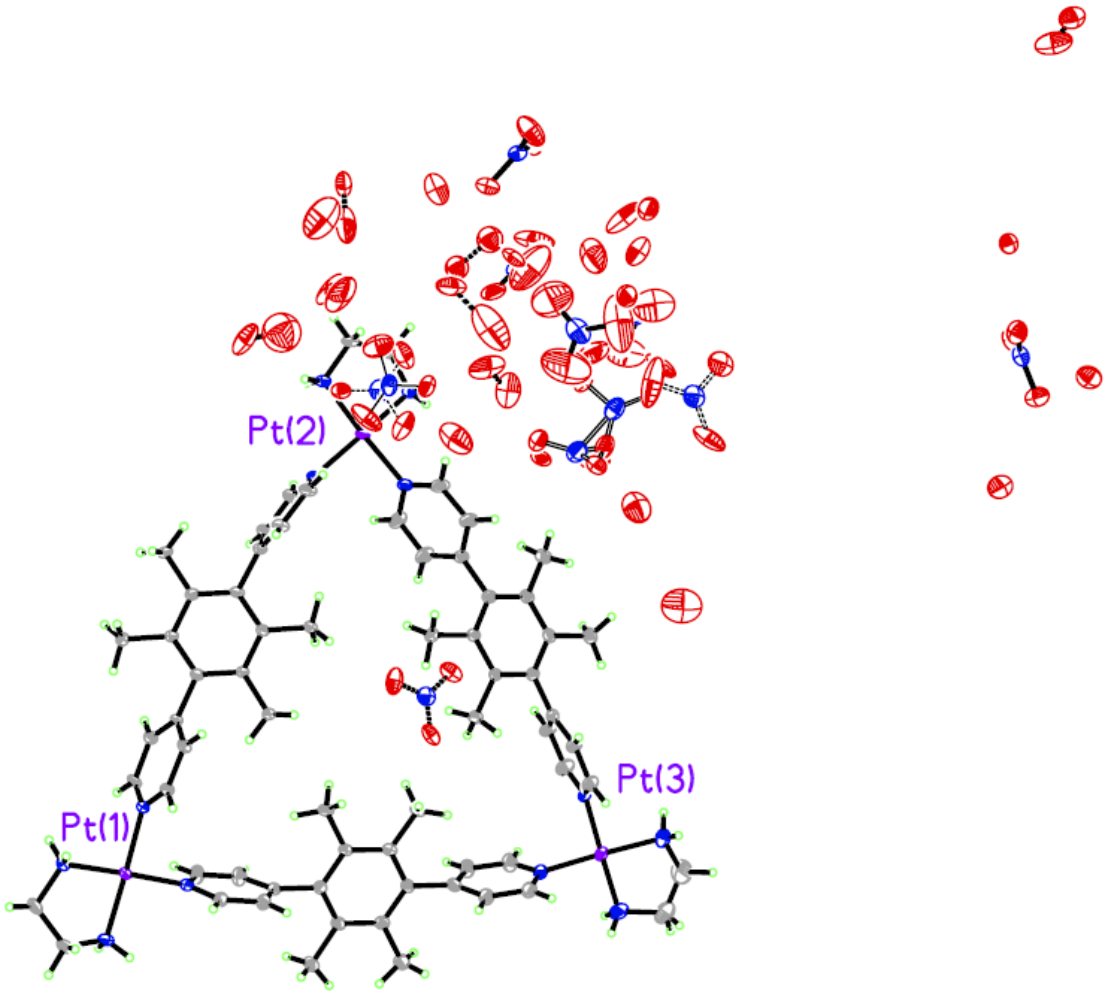

Figure S11. ORTEP views (30% probability level) of **5**·$(H_2O)_m$. Water molecules and nitrate anions are severely disordered.