Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Multicenter interactions and ligand field effects in platinum(II) tripyrrindione radicals

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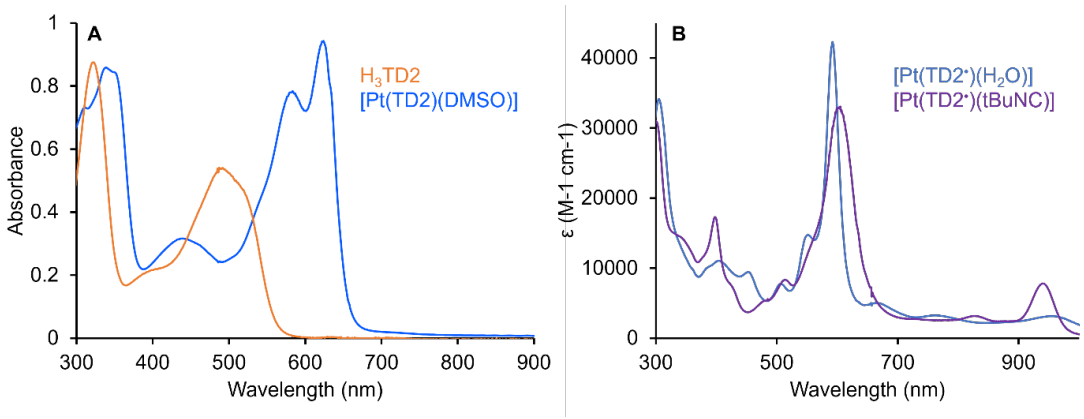

Figure S1. Optical absorption spectra of (A) H_3TD2 free ligand and the reaction mixture containing a tentative [Pt(TD2)(DMSO)] intermediate in DMSO, and (B) isolated aqua and isocyanide neutral radical complexes in CH_2Cl_2.

Table S1. X-ray crystallography details

Complex	[Pt(TD2•)(H_2O)]	[Pt(TD2•)(tBuNC)]	[Pt($TD2_{ox}$)(H_2O)][BF_4]	[Pt($TD2_{ox}$)(tBuNC)][BF_4]
Molecular Formula	$C_{24}H_{30}N_3O_3Pt$	$C_{29}H_{37}N_4O_2Pt$	$C_{24}H_{30}BF_4N_3O_3Pt$	$C_{29}H_{37}BF_4N_4O_2Pt$
Formula weight [g · mol^{-1}]	603.60	668.71	690.41	755.52
Temperature [K]	101.38	100.01	102.25	100.0
Crystal Class	monoclinic	monoclinic	triclinic	monoclinic
Space Group	$P2_1/n$	$P2_1/c$	P-1	$P2_1/n$
a [Å]	10.982(2)	11.4084(9)	12.453(4)	13.0550(4)
b [Å]	14.662(4)	9.6436(6)	15.634(5)	9.2569(3)
c [Å]	14.409(3)	25.018(2)	16.230(5)	24.1295(7)
α [°]	90	90	118.240(9)	90
β [°]	111.249(8)	101.878(4)	110.211(10)	95.9540(10)
γ [°]	90	90	92.715(10)	90
Volume [$Å^3$]	2162.4(9)	2693.5(3)	2526.0(14)	2900.29(15)
Z	4	4	4	4
ρ_{calc} [g · cm^{-3}]	1.854	1.649	1.815	1.730
μ [mm^{-1}]	6.521	5.242	5.616	4.898
F (000)	1188.0	1332.0	1352.0	1496.0
Crystal Size [mm]	0.367 × 0.123 × 0.085	0.135 × 0.138 × 0.087	0.249 × 0.075 × 0.073	0.285 × 0.119 × 0.089
Measure Reflections	25443	25951	50027	33463
Independent Reflections, I > 2σ[*I*]	4645	4756	10465	5947
R_{int}	0.0461	0.0642	0.0331	0.0270
Goodness-of-fit on F^2	1.024	1.013	1.034	1.055
Final *R* indexes for *I* > 2σ[*I*]	$R_1{}^a$ = 0.0217, $wR_2{}^b$ = 0.0504	$R_1{}^a$ = 0.0292, $wR_2{}^b$ = 0.0599	$R_1{}^a$ = 0.0303, $wR_2{}^b$ = 0.0732	$R_1{}^a$ = 0.0218, $wR_2{}^b$ = 0.0488
Final *R* indexes for all data	$R_1{}^a$ = 0.0280, $wR_2{}^b$ = 0.0531	$R_1{}^a$ = 0.0456, wR_{2b} = 0.0654	$R_1{}^a$ = 0.0383, $wR_2{}^b$ = 0.0767	$R_1{}^a$ = 0.0242, $wR_2{}^b$ = 0.0498
Peak/hole [e·$Å^{-3}$]	1.21/-0.91	0.77/-0.44	3.39/-1.09	1.31/-0.59
CCDC Number	2182028	2182030	2182029	2182027

$^a R_1 = \Sigma[|F_o| - |F_c|]/\Sigma|F_o|$ $^b wR_2 = [\Sigma w(F_o^2 - F_c^2)/\Sigma wF_o^4]^{1/2}$

Table S2. Selected bond lengths for Pt-TD2 complexes; lengths highlighted in blue show the most significant differences between redox states.

	[Pt(TD2$^{\bullet}$)(H_2O)]	[Pt($TD2_{ox}$)(H_2O)]$^{+}$	[Pt(TD2$^{\bullet}$)(tBuNC)]	[Pt($TD2_{ox}$)(tBuNC)]$^{+}$
Pt1 – N1	1.997(3)	1.992(4)	2.042(4)	1.998(2)
Pt1 – N2	1.971(3)	1.970(4)	2.036(4)	2.027(2)
Pt1 – N3	2.004(3)	2.003(4)	2.039(4)	2.006(2)
Pt1 – O3/C25	2.037(2)	2.045(3)	1.920(6)	1.952(3)
N1 – C1	1.384(4)	1.450(6)	1.369(6)	1.454(4)
N1 – C4	1.381(4)	1.336(6)	1.416(6)	1.336(4)
N2 – C6	1.373(4)	1.378(6)	1.389(6)	1.377(4)
N2 – C9	1.368(4)	1.371(6)	1.382(6)	1.367(4)
N3 – C11	1.378(4)	1.336(6)	1.383(6)	1.345(4)
N3 – C14	1.382(4)	1.437(6)	1.406(6)	1.450(4)
O1 – C1	1.243(4)	1.206(5)	1.235(6)	1.202(3)
O2 – C14	1.247(4)	1.210(5)	1.226(7)	1.207(4)
C1 – C2	1.473(4)	1.478(7)	1.485(7)	1.491(4)
C2 – C3	1.347(5)	1.333(7)	1.329(7)	1.344(4)
C3 – C4	1.467(4)	1.485(7)	1.478(7)	1.488(4)
C4 – C5	1.373(5)	1.395(7)	1.372(7)	1.396(4)
C5 – C6	1.391(4)	1.367(7)	1.401(7)	1.373(4)
C6 – C7	1.448(5)	1.458(7)	1.438(7)	1.461(4)
C7 – C8	1.357(4)	1.352(7)	1.376(7)	1.351(4)
C8 – C9	1.437(5)	1.468(7)	1.452(7)	1.474(4)
C9 – C10	1.400(4)	1.376(7)	1.399(7)	1.387(4)
C10 – C11	1.367(4)	1.387(7)	1.351(7)	1.391(4)
C11 – C12	1.466(4)	1.488(7)	1.471(7)	1.493(4)
C12 – C13	1.346(5)	1.332(7)	1.335(7)	1.336(4)
C13 – C14	1.472(4)	1.481(7)	1.508(7)	1.450(4)
N4 – C25	--	--	1.170(6)	1.155(4)
N4 – C26	--	--	1.462(7)	1.470(4)

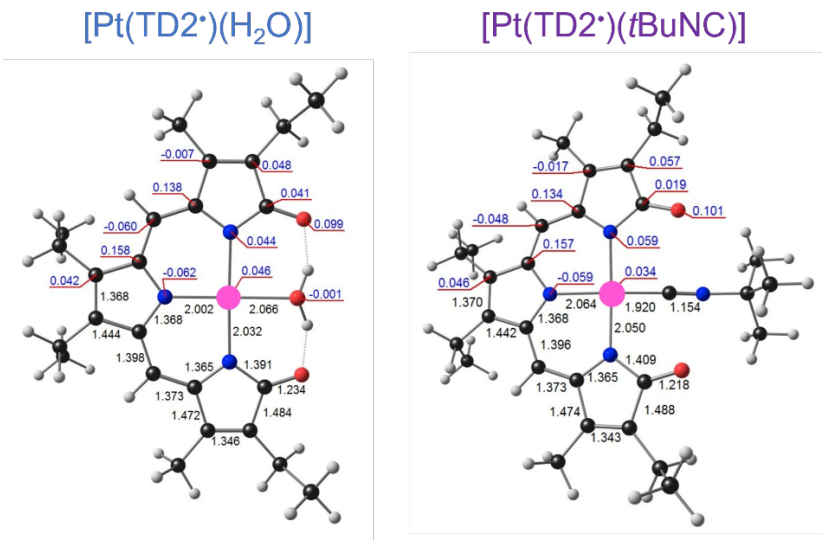

Figure S2. B3LYP-D3 optimized geometries and Mulliken spin populations for neutral radical Pt(II) tripyrrindione complexes. Calculated bond distances (Å) and spin populations are indicated in black and blue (with underlining), respectively.

EPR simulations including dynamic spin exchange

Consider an EPR spectrum of paramagnetic centers in liquid solution, which are participating in a dynamic spin exchange interaction. The shape of the EPR spectrum as a function the angular frequency, *w*, is in this case described by the following equation (see J. N. Molin, K. M. Salikhov and K. I. i. Zamaraev, *Spin exchange: Principles and applications in chemistry and biology*, Springer, 1980):

$$g(\omega) \propto \mathrm{Im}\left[\frac{iG}{1 + V_{ex}G}\right] \tag{S1}$$

where:

$$G = \sum_k \left[\frac{\varphi_k}{i(\omega_k - \omega) - \frac{1}{T_2} - V_{ex}}\right] \tag{S2}$$

In these expressions:

- V_{ex} is the spin exchange coherence transfer rate: $V_{ex} = k_{ex}C$, where k_{ex} is the spin exchange rate constant and C is the concentration of the paramagnetic center,
- φ_k are the statistical weights of EPR lines,
- ω_k are the EPR resonance frequencies that are expressed through the electronic g-factor, magnetic field, and the hyperfine constants (e.g., for an electron interacting with a single

nucleus of spin $I = 1/2$, $\omega_k = 2p(g\beta B_o \pm a_{iso}/2)/h$, where g is the electronic g-factor, β is the Bohr magneton, B_o is the magnetic field, a_{iso} is the isotropic hyperfine interaction constant, and h is the Planck constant).

- T_2 is the transverse relaxation time.

Calculations using Eqs. (S1,S2) show that the shape of the room-temperature EPR spectrum of [Pt(TD2$^{\bullet}$)(H_2O)] can be approximately reproduced for ^{195}Pt $a_{iso} < 2$ mT, $T_2 \sim 10$ ns, and $V_{ex} < 10^8$ s^{-1}. As an example, the black upper trace in Figure 3 in the main text shows the simulation for ^{195}Pt $a_{iso} = 1.4$ mT, $T_2 = 10.5$ ns, and $V_{ex} = 4 \cdot 10^7$ s^{-1} (see the detailed parameters in Table S3).

Table S3. EPR simulation parameters for Figure 3

Complex / measurement temperature / phase state	***EPR simulation parameters***
[Pt(TD2$^{\bullet}$)(H_2O)] / 298 K (room temperature) / liquid (Fig. 2a, top black trace)	$g = 2.004$; $a_{iso}(^{195}Pt) = 1.4$ mT; $T_2 = 10.5$ ns; Gaussian width, 0.6 mT; $V_{ex} = 4 \cdot 10^7$ s^{-1} (~0.23 mT)
[Pt(TD2$^{\bullet}$)(tBuNC)] / 298 K (room temperature) / liquid (Fig. 2a, bottom black trace)	$g = 2.006$; $a_{iso}(^{195}Pt) = 2.2$ mT; $T_2 = 50$ ns; Gaussian width, 0.6 mT; $V_{ex} = 0$
[Pt(TD2$^{\bullet}$)(H_2O)] / 77 K / frozen glassy solution (Fig. 2b, top black trace)	$(g_1, g_2, g_3) = (2.026, 2.016, 1.968)$ Individual Gaussian linewidths: $(\delta B_1, \delta B_2, \delta B_3) = (1, 0.8, 1.1)$ mT Because of low signal/noise ratio, the ^{195}Pt hfi was not accounted for (effectively included into the individual linewidth)
[Pt(TD2$^{\bullet}$)(tBuNC)] 77 K / frozen glassy solution (Fig. 2b, bottom black trace)	$(g_1, g_2, g_3) = (2.022, 2.014, 1.978)$ ^{195}Pt hfi splittings: $(A_1, A_2, A_3) = (2.15, 1.99, 2.49)$ mT Individual Gaussian linewidths: $(\delta B_1, \delta B_2, \delta B_3) = (0.7, 0.55, 1.1)$ mT for the component without ^{195}Pt hfi and $(\delta B_1, \delta B_2, \delta B_3) = (0.9, 0.55, 1.1)$ mT for the component with ^{195}Pt hfi

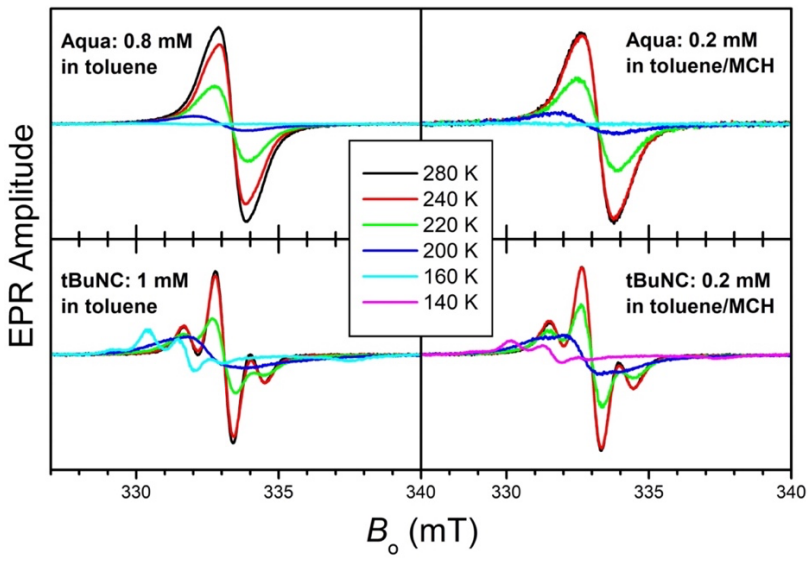

Figure S3. Variable-temperature EPR spectra of [Pt(TD2$^{\bullet}$)(H_2O)] and [Pt(TD2$^{\bullet}$)(*t*BuNC)] in toluene or in toluene/methylcyclohexane (1:3 *v/v*).

Table S4. Half-wave potentials of divalent metal complexes of tripyrrin-1,14-dione in CH_2Cl_2

Complex	$E_{1/2}$ ox. (V vs Fc/Fc^+)	$E_{1/2}$ red. (V vs Fc/Fc^+)
[Pd(TD1$^{\bullet}$)(H_2O)]	–0.052	–0.672
[Cu(TD1$^{\bullet}$)(H_2O)]	–0.052	–0.688
[Pt(TD2$^{\bullet}$)(H_2O)]	–0.107	–0.701
[Pt(TD2$^{\bullet}$)(tBuNC)]	–0.338	–0.866

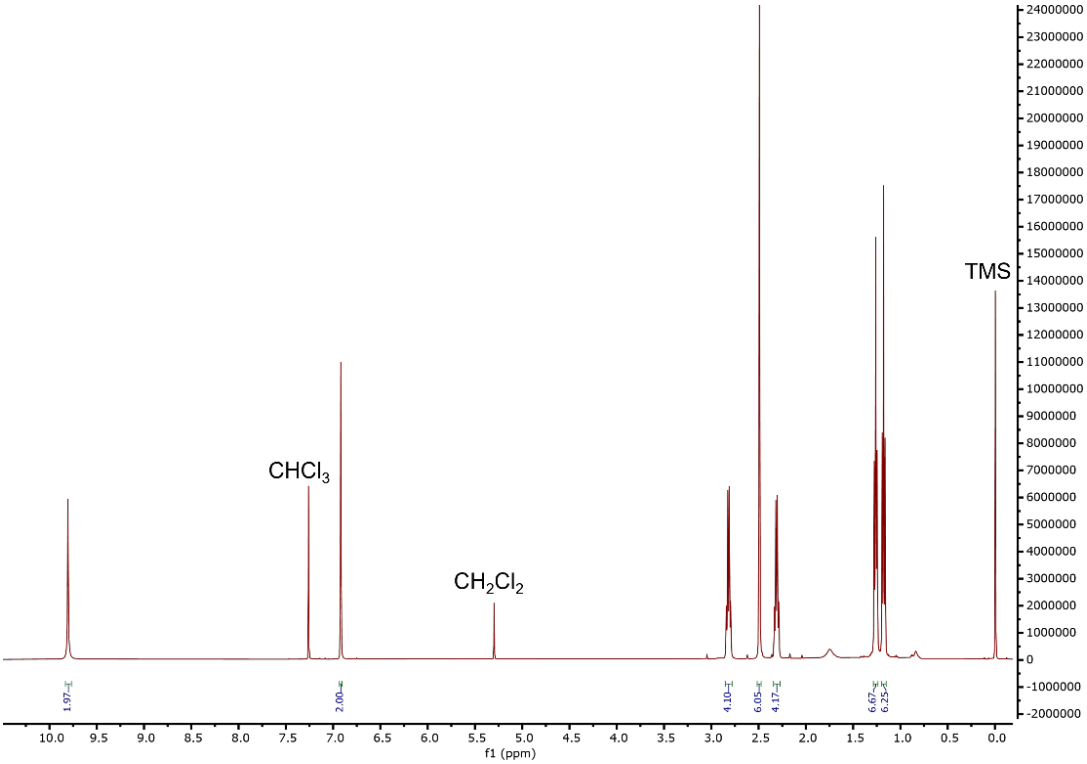

Figure S4. ^{1}H NMR spectrum of $[Pt(TD2_{ox})(H_2O)][BF_4]$ in $CDCl_3$ at 298 K.

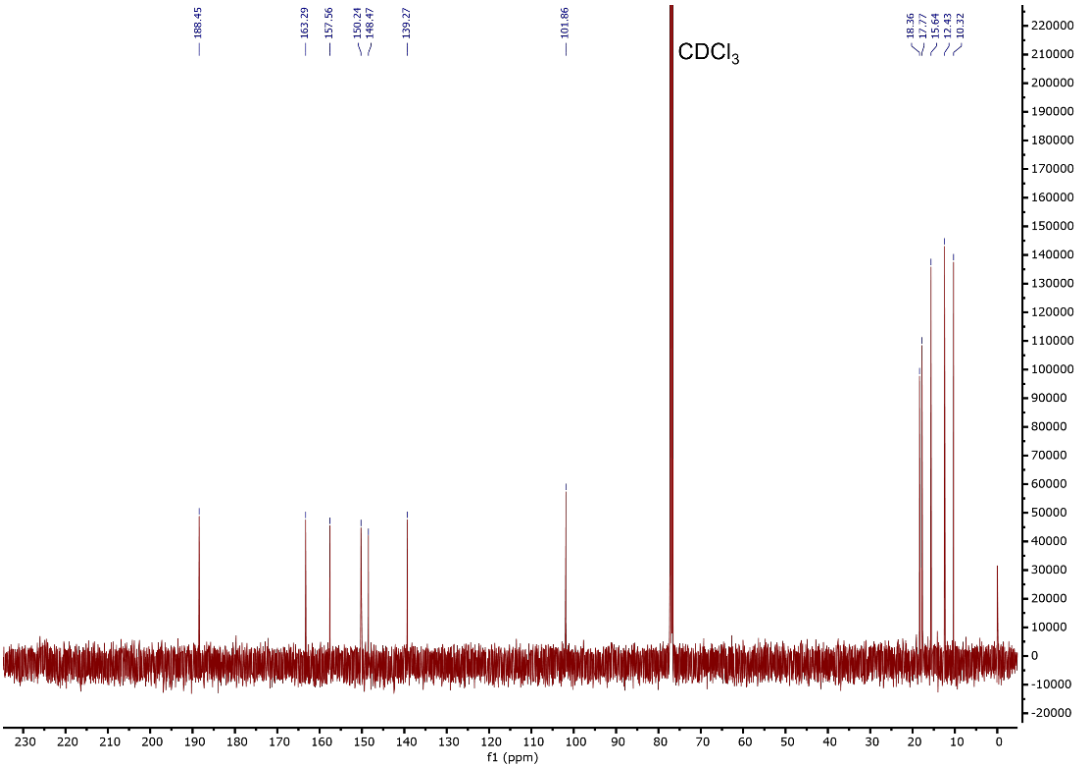

Figure S5. ^{13}C NMR spectrum of $[Pt(TD2_{ox})(H_2O)][BF_4]$ in $CDCl_3$ at 298 K.

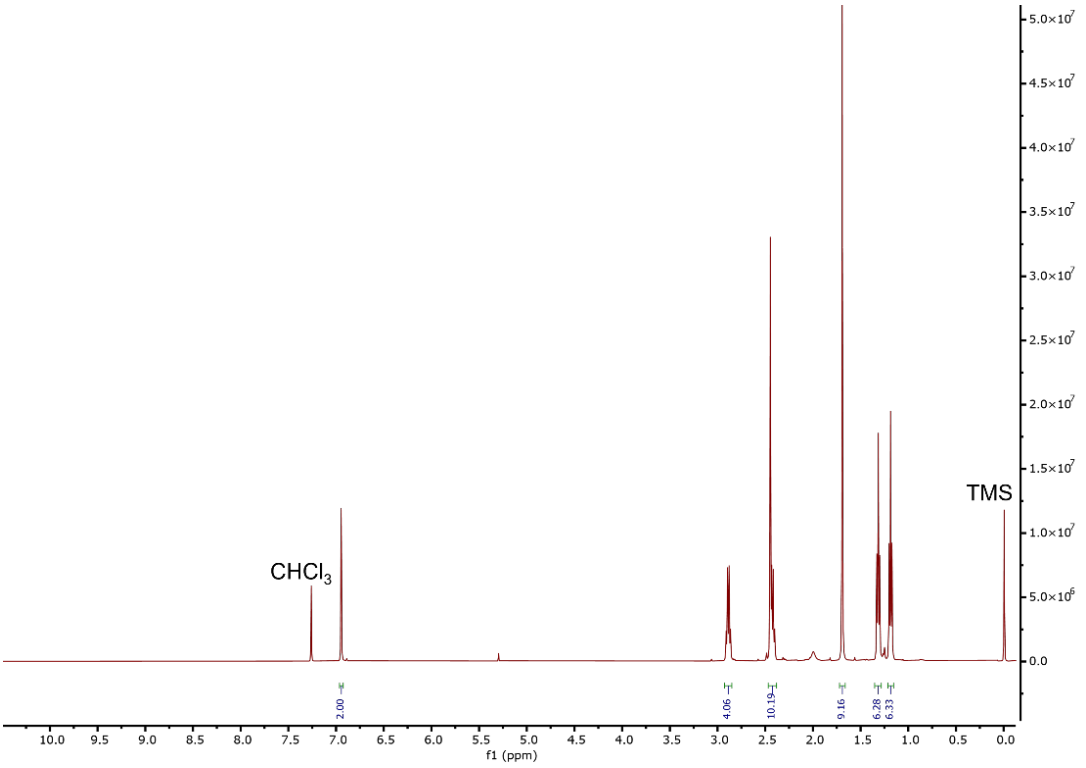

Figure S6. ^{1}H NMR spectrum of [Pt(TD2$_{ox}$)(*t*BuNC)][BF_4] in $CDCl_3$ at 298 K.

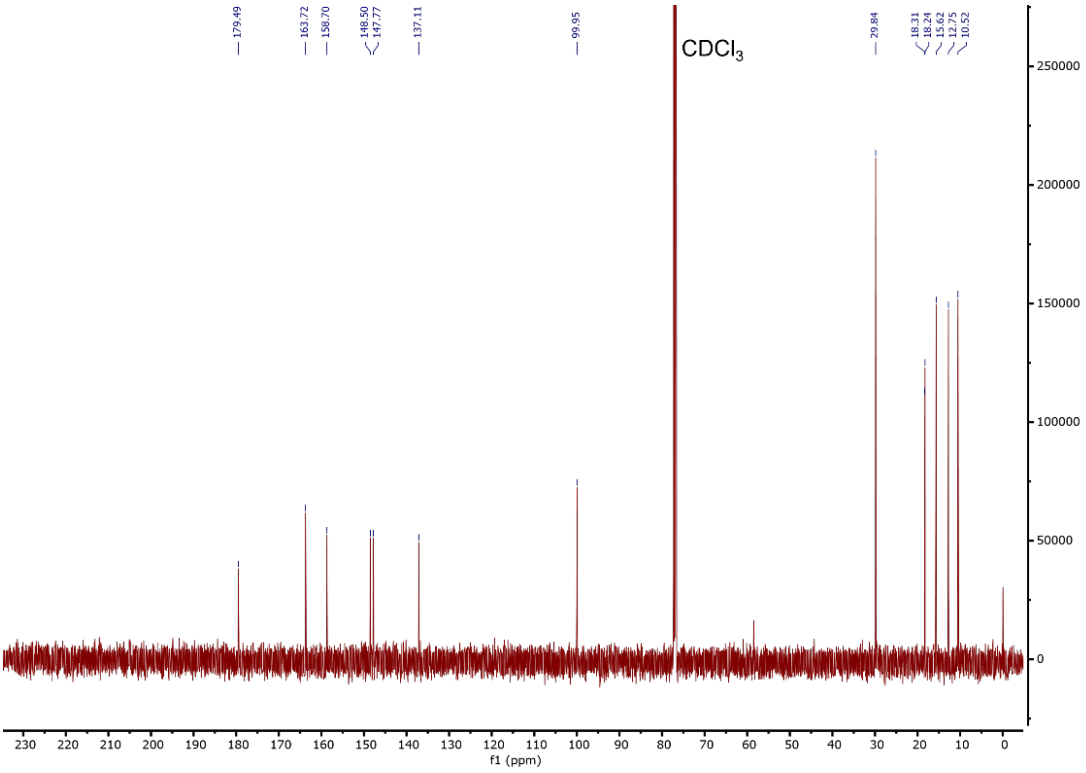

Figure S7. ^{13}C NMR spectrum of [Pt(TD2$_{ox}$)(*t*BuNC)][BF_4] in $CDCl_3$ at 298 K.

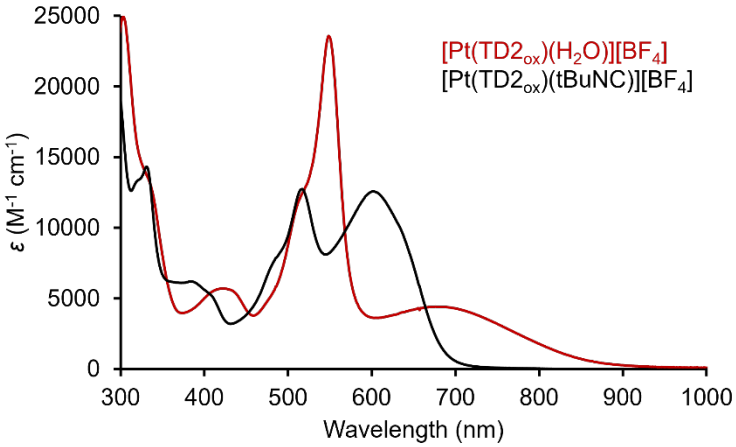

Figure S8. UV-visible absorption spectra of $[Pt(TD2_{ox})(H_2O)][BF_4]$ (red) and $[Pt(TD2_{ox})(t\text{BuNC})][BF_4]$ (black) in CH_2Cl_2.

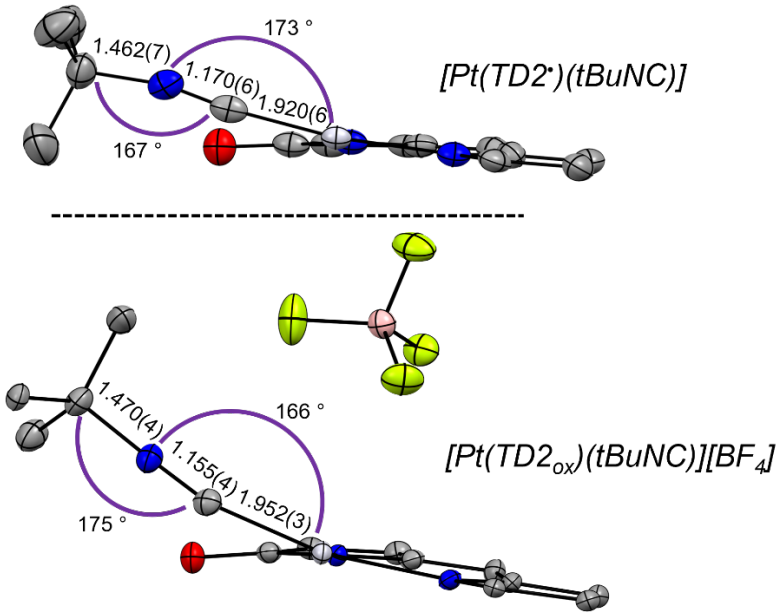

Figure S9. Comparison of isocyanide bond lengths and angles between the neutral and cationic Pt(II) tripyrrindione complexes.

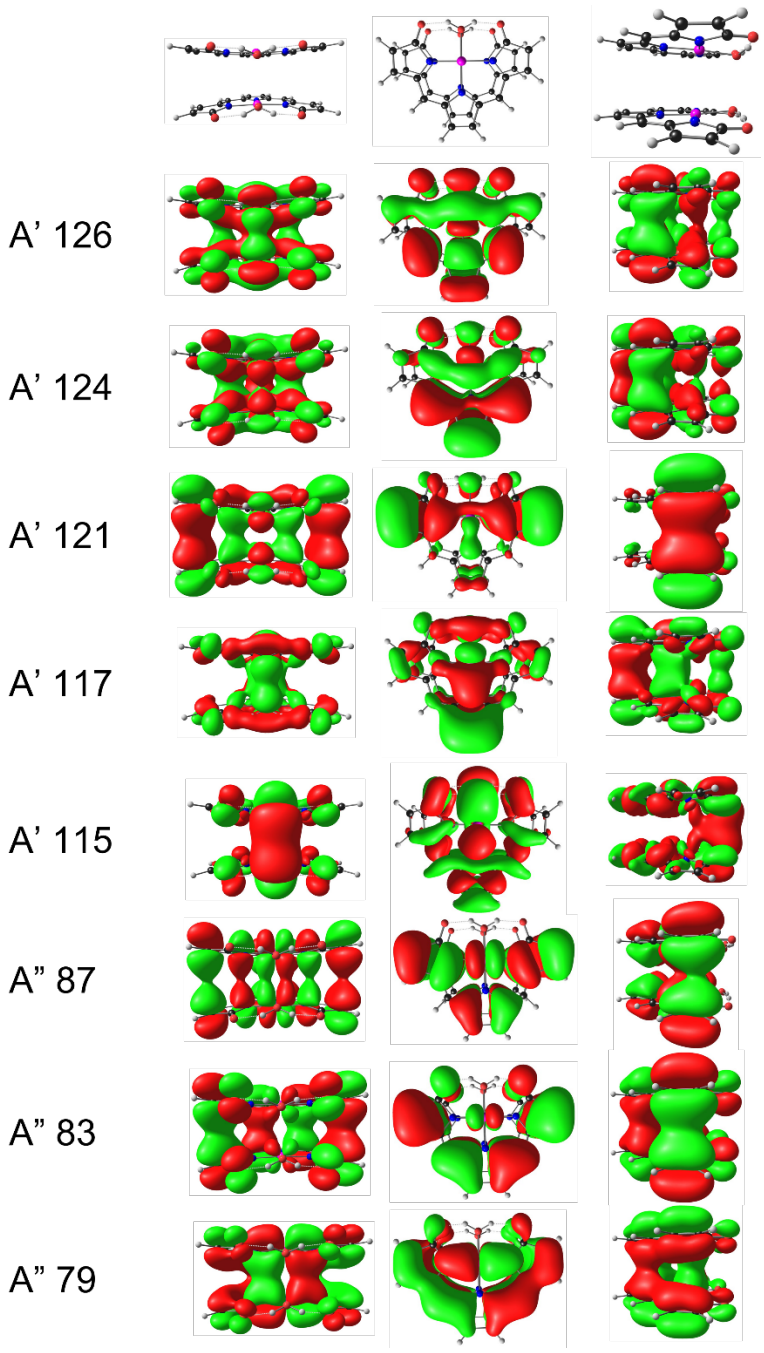

Figure S10. B3LYP-D3 calculated valence MOs of $[Pt(TD2'_{ox})(H_2O)]_2^{2+}$ (C_s).

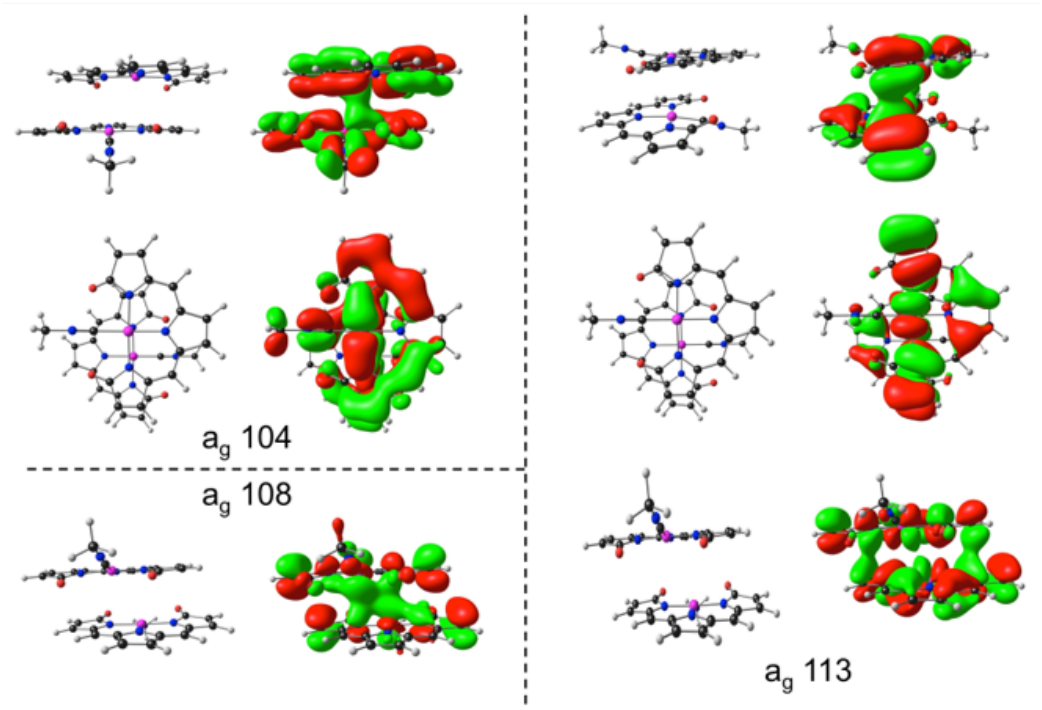

Figure S11. B3LYP-D3 calculated valence MOs of $[Pt(TD2'_{ox})(MeNC)]_2^{2+}$ (C_i).

Optimized Cartesian coordinates (Å)

All compounds were optimized the ZORA Hamiltonian, ZORA/QZ4P basis set, all electron, OLYP functional.

1. [Pt(TD2)(CN^{t}Bu)], C_s, q = 0, S = 1/2

Pt	-0.046144000	0.022106000	0.000000000
C	0.042309000	-0.706700000	4.262931000
C	0.042309000	-0.706700000	-4.262931000
C	0.198939000	0.626415000	4.303295000
C	0.198939000	0.626415000	-4.303295000
C	0.236113000	1.114875000	2.898423000
C	0.236113000	1.114875000	-2.898423000
C	0.386588000	1.557363000	5.450210000
C	0.386588000	1.557363000	-5.450210000
C	0.658112000	4.961101000	0.000000000
C	1.866212000	1.901105000	5.681354000
C	1.866212000	1.901105000	-5.681354000
C	-0.027993000	-1.097785000	2.843783000
C	-0.027993000	-1.097785000	-2.843783000
C	-0.031076000	-1.675413000	5.394280000
C	-0.031076000	-1.675413000	-5.394280000
C	-0.092167000	-2.851456000	1.100060000
C	-0.092167000	-2.851456000	-1.100060000
C	-0.100700000	-2.401855000	2.421482000
C	-0.100700000	-2.401855000	-2.421482000
C	-0.182773000	-4.229225000	0.684902000
C	-0.182773000	-4.229225000	-0.684902000
C	-0.314321000	-5.397221000	1.609382000
C	-0.314321000	-5.397221000	-1.609382000
C	-0.368137000	1.914520000	0.000000000
C	-0.789119000	4.448069000	0.000000000
C	-1.529461000	4.887399000	1.268028000

C	-1.529461000	4.887399000	-1.268028000
C	-1.750586000	-5.604011000	2.114830000
C	-1.750586000	-5.604011000	-2.114830000
H	0.007637000	-1.162236000	6.353078000
H	0.007637000	-1.162236000	-6.353078000
H	0.019429000	-6.302291000	1.099219000
H	0.019429000	-6.302291000	-1.099219000
H	0.354333000	-5.269853000	2.464268000
H	0.354333000	-5.269853000	-2.464268000
H	0.655548000	6.051375000	0.000000000
H	0.799222000	-2.384742000	5.361246000
H	0.799222000	-2.384742000	-5.361246000
H	1.180294000	4.603981000	0.886159000
H	1.180294000	4.603981000	-0.886159000
H	1.976136000	2.606531000	6.506232000
H	1.976136000	2.606531000	-6.506232000
H	2.293401000	2.350975000	4.785662000
H	2.293401000	2.350975000	-4.785662000
H	2.439298000	1.003641000	5.918869000
H	2.439298000	1.003641000	-5.918869000
H	-0.039941000	1.125365000	6.357373000
H	-0.039941000	1.125365000	-6.357373000
H	-0.155199000	-3.159862000	3.188372000
H	-0.155199000	-3.159862000	-3.188372000
H	-0.160960000	2.478828000	5.241351000
H	-0.160960000	2.478828000	-5.241351000
H	-0.954969000	-2.257057000	5.358671000
H	-0.954969000	-2.257057000	-5.358671000
H	-1.013794000	4.513976000	2.151095000

H	-1.013794000	4.513976000	-2.151095000
H	-1.567068000	5.976133000	1.305516000
H	-1.567068000	5.976133000	-1.305516000
H	-1.805998000	-6.453865000	2.796879000
H	-1.805998000	-6.453865000	-2.796879000
H	-2.110298000	-4.718892000	2.640252000
H	-2.110298000	-4.718892000	-2.640252000
H	-2.428508000	-5.790035000	1.281300000
H	-2.428508000	-5.790035000	-1.281300000
H	-2.549922000	4.504323000	1.269457000
H	-2.549922000	4.504323000	-1.269457000
N	0.045747000	0.007887000	2.047452000
N	0.045747000	0.007887000	-2.047452000
N	-0.021144000	-2.042197000	0.000000000
N	-0.723671000	3.011908000	0.000000000
O	0.419218000	2.269655000	2.557156000
O	0.419218000	2.269655000	-2.557156000

2. [Pt(TD2)(OH_2)], C_s, q = 0, S = 1/2

C	0.708530000	-4.285060000	-0.173191000
C	1.119259000	-2.906669000	-0.043217000
C	1.641123000	-5.443179000	-0.333085000
C	2.160181000	-5.600856000	-1.771106000
C	2.441438000	-2.453817000	-0.001354000
C	2.829236000	1.066362000	0.189001000
C	2.854269000	-1.149070000	0.103507000
C	4.247218000	0.642994000	0.075308000

C	4.255110000	-0.702273000	0.032224000
C	5.358327000	1.633766000	0.048070000
C	5.414362000	-1.632282000	-0.083628000
C	5.669579000	2.199372000	1.442473000
C	-0.659629000	-4.293519000	-0.173005000
C	-1.087234000	-2.919979000	-0.045091000
C	-1.578359000	-5.462843000	-0.331555000
C	-2.096465000	-5.627717000	-1.769116000
C	-2.414831000	-2.482707000	-0.005576000
C	-2.843205000	-1.183085000	0.100407000
C	-2.845566000	1.032131000	0.195233000
C	-4.249377000	-0.753166000	0.029478000
C	-4.258017000	0.591895000	0.078378000
C	-5.380739000	1.569611000	0.053128000
C	-5.397140000	-1.696676000	-0.091254000
C	-5.696447000	2.132248000	1.447663000
H	0.831834000	2.288646000	0.508339000
H	1.133176000	-6.360927000	-0.033116000
H	1.333493000	-5.770809000	-2.461419000
H	2.488922000	-5.332599000	0.347360000
H	2.682893000	-4.701736000	-2.098551000
H	2.848149000	-6.444157000	-1.846660000
H	3.211577000	-3.205730000	-0.087618000
H	4.785888000	2.678027000	1.863207000
H	5.071597000	2.456616000	-0.610305000
H	5.342628000	-2.242589000	-0.986952000
H	5.454618000	-2.316826000	0.766730000
H	5.984099000	1.405216000	2.121031000
H	6.254164000	1.177726000	-0.376528000

H	6.355280000	-1.087357000	-0.119506000
H	6.467744000	2.940771000	1.388484000
H	-0.861364000	2.278718000	0.510239000
H	-1.059389000	-6.374286000	-0.031210000
H	-1.268264000	-5.788223000	-2.459888000
H	-2.426996000	-5.361761000	0.349325000
H	-2.630092000	-4.735130000	-2.096829000
H	-2.774375000	-6.479216000	-1.843637000
H	-3.175903000	-3.243580000	-0.093780000
H	-4.817229000	2.619959000	1.867332000
H	-5.104290000	2.395694000	-0.605697000
H	-5.316103000	-2.303614000	-0.996052000
H	-5.431188000	-2.383969000	0.757175000
H	-6.002344000	1.335187000	2.126741000
H	-6.271836000	1.103362000	-0.370319000
H	-6.344404000	-1.162895000	-0.127809000
H	-6.502027000	2.865612000	1.394118000
N	0.011058000	-2.108115000	0.022793000
N	2.028427000	-0.069937000	0.231788000
N	-2.030607000	-0.094264000	0.232138000
O	2.436400000	2.235729000	0.217539000
O	-0.011938000	1.873514000	0.826944000
O	-2.467488000	2.206290000	0.231103000
Pt	-0.000829000	-0.126957000	0.310100000

3. [Pt(TD2)(CN^{t}Bu)]$_2$ simplified, C_1, q = 0 (BS), S = 0

C	0.090800000	5.605700000	13.221500000
C	0.337100000	2.359500000	7.902300000
C	0.704500000	5.522300000	14.447500000
C	1.139300000	8.956800000	12.122400000
C	1.229700000	2.984400000	10.201000000
C	1.314100000	9.092000000	13.440600000
C	1.806300000	4.733100000	14.759600000
C	2.066500000	7.454900000	10.362800000
C	2.075800000	7.944500000	11.646200000
C	2.393600000	8.164500000	13.851100000
C	2.479100000	4.703000000	16.025200000
C	2.801200000	5.878400000	8.547900000
C	2.865700000	6.426900000	9.871400000
C	3.390900000	3.212700000	14.611700000
C	3.457800000	3.763600000	15.934000000
C	3.780300000	4.939400000	8.456900000
C	3.862200000	1.473500000	10.632800000
C	4.178400000	1.692900000	12.838000000
C	4.188000000	2.182700000	14.121400000
C	4.450900000	4.907000000	9.724100000
C	4.939800000	0.543900000	11.044400000
C	5.029800000	6.662100000	14.279800000
C	5.114500000	0.679700000	12.362900000
C	5.551400000	4.116200000	10.038100000
C	5.941600000	7.309800000	16.565300000
C	6.164000000	4.032600000	11.264700000
C	6.590200000	4.162800000	13.458000000

C	7.253700000	3.106900000	11.551100000
C	7.513100000	3.170100000	12.861500000
C	-0.335300000	5.479000000	11.028400000
C	-1.000000000	6.530300000	12.937200000
C	-1.259400000	6.469500000	11.626800000
H	0.329700000	6.165900000	15.230200000
H	0.423500000	9.447400000	11.482400000
H	0.795400000	9.724400000	14.141500000
H	1.201600000	2.068000000	7.305900000
H	1.339400000	7.873300000	9.681800000
H	2.081800000	6.174300000	7.803200000
H	2.230400000	5.336700000	16.859700000
H	4.030100000	4.306800000	7.622000000
H	4.177700000	3.468000000	16.678400000
H	4.914500000	1.763700000	14.802600000
H	5.084500000	7.613500000	17.166400000
H	5.457600000	-0.089500000	10.343800000
H	5.829600000	0.188900000	13.003400000
H	5.926300000	3.471900000	9.256000000
H	6.378400000	6.395900000	16.968300000
H	6.688100000	8.102500000	16.575100000
H	7.703300000	2.474100000	10.802800000
H	8.231500000	2.621400000	13.447100000
H	-0.100400000	3.276700000	7.507900000
H	-0.405100000	1.563100000	7.874600000
H	-1.450000000	7.161300000	13.686800000
H	-1.978600000	7.018300000	11.042300000
N	0.442900000	4.943800000	12.081900000
N	0.752400000	2.590400000	9.228300000

N	2.398900000	3.839400000	13.909400000
N	2.855400000	7.517400000	12.679800000
N	3.399600000	2.120600000	11.803900000
N	3.857500000	5.800200000	10.574100000
N	5.512700000	7.063500000	15.246500000
N	5.812600000	4.696300000	12.403300000
O	2.792200000	7.968700000	14.984400000
O	3.465100000	1.669700000	9.499100000
O	6.492500000	4.446700000	14.638100000
O	-0.237700000	5.198000000	9.847600000
Pt	1.873000000	3.481600000	11.939400000
Pt	4.383300000	6.158900000	12.544400000

4. [Pt(TD2)(OH$_2$)]$_2$ simplified, C_1, q = 0 (BS), S = 0

C	0.411200000	5.502500000	14.080000000
C	1.360600000	8.971500000	12.605900000
C	1.473600000	4.678800000	14.455000000
C	1.748700000	9.210600000	13.865600000
C	2.067600000	4.624800000	15.761000000
C	2.127900000	7.412600000	10.795400000
C	2.205100000	7.907300000	12.073400000
C	2.817200000	5.871200000	8.927700000
C	2.862700000	8.288500000	14.165900000
C	2.950200000	6.429600000	10.244700000
C	3.069500000	3.712100000	15.708400000
C	3.102300000	3.192300000	14.370300000
C	3.654900000	1.434600000	10.443000000

C	3.789400000	4.933700000	8.789300000
C	3.985700000	2.221500000	13.897000000
C	4.025800000	1.720000000	12.619200000
C	4.532600000	4.908300000	10.018200000
C	4.789200000	0.571500000	10.825500000
C	5.006800000	0.753600000	12.135000000
C	5.620000000	4.078200000	10.291100000
C	6.316800000	4.023900000	11.472100000
C	7.020000000	4.444000000	13.542500000
C	7.497700000	3.198000000	11.704800000
C	7.932400000	3.446000000	12.947600000
C	-0.143900000	5.583500000	12.827100000
C	-0.473800000	5.339900000	10.639500000
C	-1.181900000	6.531900000	12.437700000
C	-1.388100000	6.394500000	11.120700000
H	0.013700000	6.159300000	14.841000000
H	0.579900000	9.452500000	12.038700000
H	0.634000000	3.656800000	9.394100000
H	1.351600000	7.809100000	10.156400000
H	1.377000000	9.929800000	14.575700000
H	1.763600000	5.234800000	16.595000000
H	1.846400000	2.487800000	9.340700000
H	2.050100000	6.149200000	8.225100000
H	3.751900000	3.424500000	16.490300000
H	3.985500000	4.291100000	7.947700000
H	4.580700000	7.028500000	15.186900000
H	4.717600000	1.847300000	14.599100000
H	5.310700000	-0.055800000	10.122300000
H	5.764500000	0.308200000	12.759600000

H	5.846300000	5.899000000	14.990700000
H	5.937400000	3.418200000	9.496300000
H	7.911800000	2.529200000	10.967200000
H	8.781900000	3.043300000	13.472700000
H	-1.654700000	7.214400000	13.125900000
H	-2.066300000	6.922500000	10.471900000
N	0.233800000	4.850800000	11.739000000
N	2.126200000	3.802800000	13.631100000
N	3.084300000	7.500000000	13.035300000
N	3.201000000	2.082700000	11.593900000
N	4.000500000	5.827100000	10.881400000
N	6.035800000	4.742800000	12.597800000
O	1.067700000	2.873200000	9.820200000
O	3.210300000	1.588000000	9.302200000
O	3.491100000	8.230600000	15.226600000
O	4.904300000	6.162800000	14.823100000
O	7.115000000	4.932100000	14.671500000
O	-0.331400000	4.980900000	9.467400000
Pt	1.680100000	3.423800000	11.716600000
Pt	4.508800000	6.067700000	12.803200000

5. [Pt(TD2)(CN^{t}Bu)]$_2^{2+}$ simplified, C_i, q = 2, S = 0

C	0.524863000	-2.764069000	-4.653003000
C	0.583630000	-1.515427000	-3.852114000
C	0.871510000	-3.766661000	-3.851871000
C	1.195356000	-3.206558000	-2.522209000
C	1.485454000	-3.999709000	-1.418705000

C	1.618069000	0.903536000	-2.268943000
C	1.700577000	-3.526039000	-0.142202000
C	1.764322000	2.083753000	0.570175000
C	1.966757000	-4.360101000	1.022060000
C	2.003806000	2.814912000	-3.934460000
C	2.051641000	-2.173067000	1.553759000
C	2.177600000	-3.533267000	2.059032000
C	2.185496000	2.537896000	1.919329000
C	2.194172000	0.265363000	1.799949000
C	2.275729000	-1.032859000	2.291655000
C	2.426012000	1.453645000	2.648261000
C	-0.524863000	2.764069000	4.653003000
C	-0.583630000	1.515427000	3.852114000
C	-0.871510000	3.766661000	3.851871000
C	-1.195356000	3.206558000	2.522209000
C	-1.485454000	3.999709000	1.418705000
C	-1.618069000	-0.903536000	2.268943000
C	-1.700577000	3.526039000	0.142202000
C	-1.764322000	-2.083753000	-0.570175000
C	-1.966757000	4.360101000	-1.022060000
C	-2.003806000	-2.814912000	3.934460000
C	-2.051641000	2.173067000	-1.553759000
C	-2.177600000	3.533267000	-2.059032000
C	-2.185496000	-2.537896000	-1.919329000
C	-2.194172000	-0.265363000	-1.799949000
C	-2.275729000	1.032859000	-2.291655000
C	-2.426012000	-1.453645000	-2.648261000
H	0.214888000	-2.780196000	-5.684554000
H	0.916716000	-4.821242000	-4.074561000

H	1.331167000	2.678103000	-4.779647000
H	1.515372000	-5.069302000	-1.567708000
H	1.780424000	3.748922000	-3.421229000
H	1.995738000	-5.437292000	1.004956000
H	2.243809000	3.578685000	2.189303000
H	2.422610000	-3.784403000	3.078089000
H	2.529941000	-1.151737000	3.334508000
H	2.727189000	1.386410000	3.681459000
H	3.033479000	2.827920000	-4.286974000
H	-0.214888000	2.780196000	5.684554000
H	-0.916716000	4.821242000	4.074561000
H	-1.331167000	-2.678103000	4.779647000
H	-1.515372000	5.069302000	1.567708000
H	-1.780424000	-3.748922000	3.421229000
H	-1.995738000	5.437292000	-1.004956000
H	-2.243809000	-3.578685000	-2.189303000
H	-2.422610000	3.784403000	-3.078089000
H	-2.529941000	1.151737000	-3.334508000
H	-2.727189000	-1.386410000	-3.681459000
H	-3.033479000	-2.827920000	4.286974000
N	1.092898000	-1.872573000	-2.538516000
N	1.733950000	-2.211078000	0.225168000
N	1.829958000	1.740170000	-3.026822000
N	1.871585000	0.632944000	0.556172000
N	-1.092898000	1.872573000	2.538516000
N	-1.733950000	2.211078000	-0.225168000
N	-1.829958000	-1.740170000	3.026822000
N	-1.871585000	-0.632944000	-0.556172000
O	0.211440000	-0.416068000	-4.157480000

O	1.351547000	2.747912000	-0.338219000
O	-0.211440000	0.416068000	4.157480000
O	-1.351547000	-2.747912000	0.338219000
Pt	1.528127000	-0.589537000	-1.026431000
Pt	-1.528127000	0.589537000	1.026431000

6. $[Pt(TD2)(OH_2)]_2^{2+}$ simplified, C_s, q = 2, S = 0

C	1.635755000	-3.970799000	0.671403000
C	1.635755000	-3.970799000	-0.671403000
C	1.716550000	-2.581489000	1.102825000
C	1.716550000	-2.581489000	-1.102825000
C	1.762725000	-2.159882000	2.414886000
C	1.762725000	-2.159882000	-2.414886000
C	1.878347000	-0.835319000	2.823596000
C	1.878347000	-0.835319000	-2.823596000
C	2.028401000	-0.429049000	4.239053000
C	2.028401000	-0.429049000	-4.239053000
C	2.113535000	1.381860000	2.879302000
C	2.113535000	1.381860000	-2.879302000
C	2.167890000	0.892399000	4.278659000
C	2.167890000	0.892399000	-4.278659000
C	-1.838101000	1.641496000	2.875773000
C	-1.838101000	1.641496000	-2.875773000
C	-1.992632000	1.172502000	4.274603000
C	-1.992632000	1.172502000	-4.274603000
C	-1.998030000	-0.582381000	2.823134000
C	-1.998030000	-0.582381000	-2.823134000

C	-2.087815000	-0.153002000	4.236843000
C	-2.087815000	-0.153002000	-4.236843000
C	-2.113217000	-1.906929000	2.414864000
C	-2.113217000	-1.906929000	-2.414864000
C	-2.135321000	-2.330782000	1.102752000
C	-2.135321000	-2.330782000	-1.102752000
C	-2.296002000	-3.713224000	0.671359000
C	-2.296002000	-3.713224000	-0.671359000
H	1.604562000	-4.814644000	1.340892000
H	1.604562000	-4.814644000	-1.340892000
H	1.747968000	-2.919879000	3.183025000
H	1.747968000	-2.919879000	-3.183025000
H	2.039123000	-1.130185000	5.058777000
H	2.039123000	-1.130185000	-5.058777000
H	2.071259000	2.683250000	0.832579000
H	2.071259000	2.683250000	-0.832579000
H	2.321763000	1.550346000	5.117758000
H	2.321763000	1.550346000	-5.117758000
H	-1.542515000	2.912191000	0.831848000
H	-1.542515000	2.912191000	-0.831848000
H	-2.036121000	1.849073000	5.111952000
H	-2.036121000	1.849073000	-5.111952000
H	-2.229269000	-0.839661000	5.056690000
H	-2.229269000	-0.839661000	-5.056690000
H	-2.234958000	-2.657591000	3.182696000
H	-2.234958000	-2.657591000	-3.182696000
H	-2.409882000	-4.549908000	1.340872000
H	-2.409882000	-4.549908000	-1.340872000
N	1.763162000	-1.774148000	0.000000000

N	1.904054000	0.233354000	2.020552000
N	1.904054000	0.233354000	-2.020552000
N	-1.827499000	0.472816000	2.019797000
N	-1.827499000	0.472816000	-2.019797000
N	-2.039503000	-1.527757000	0.000000000
O	1.730355000	2.286482000	0.000000000
O	2.231403000	2.519040000	2.494816000
O	2.231403000	2.519040000	-2.494816000
O	-1.277287000	2.459603000	0.000000000
O	-1.745044000	2.780547000	2.489960000
O	-1.745044000	2.780547000	-2.489960000
Pt	1.835005000	0.227946000	0.000000000
Pt	-1.754575000	0.454739000	0.000000000