Supplementary Material (ESI) for Dalton Transactions

Pt(II) Complexes of Unsubstituted Guanine and 7-Methylguanine

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Supporting Material

Figure S1. Proposed hydrogen bonded associated structure formed at basic pH due to deprotonation at N1(H) position in compound **3**.

Figure S2. pD dependence (δ, ppm) of H8 resonance for $[Pt(dien)(GH_2\text{-}N9)]^{2+}$ (**1**) in D_2O.

Figure S3. Views of two crystallographically independent cations (**1a′**, left; **1a″**, right) of $[Pt(dien)(GH_2\text{-}N9)](ClO_4)_2 \cdot 2.25\ H_2O$ (**1a**) with atom numbering scheme.

Figure S4. ^{1}H NMR spectrum presenting the formation of $[\{Pt(dien)\}_2(GH\text{-}N7,N9)]^{3+}$ (**3**) (pH* 9.80, D_2O).

Figure S5. pD dependence (δ, ppm) of H8 resonance for $[\{Pt(dien)\}_2(GH\text{-}N7,N9)]^{3+}$ (**3**) in D_2O.

Figure S6. pD dependence (δ, ppm) of H8 proton for $[Pt(dien)(7\text{-}MeGH\text{-}N9)]^{2+}$(**4**).

Figure S7. pD dependence (δ, ppm) of H8 proton for *cis*-$[Pt(NH_3)_2(7\text{-}MeGH\text{-}N9)_2]^{2+}$ (**5**).

Tables S1-S3. Calculated energies and atom coordinates of $[Pt(dien)(GH_2\text{-}N7)]^{2+}$(**2**), $[Pt(dien)(GH_2\text{-}N9)]^{2+}$ (**1**) and $[\{Pt(dien)\}_2(GH\text{-}N7,N9)]^{3+}$ (**3**) respectively.

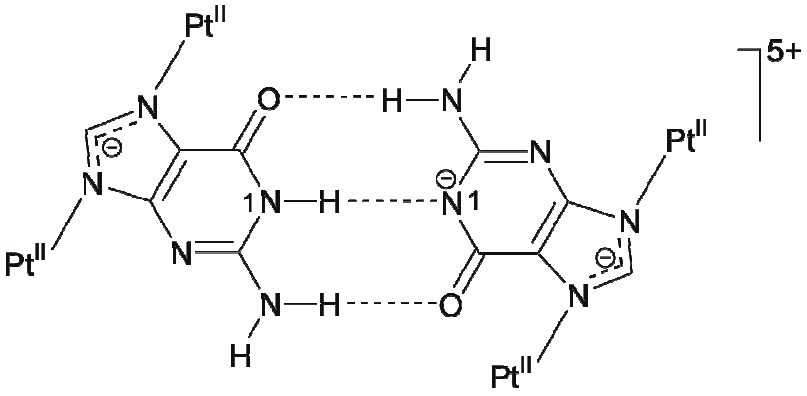

Figure S1

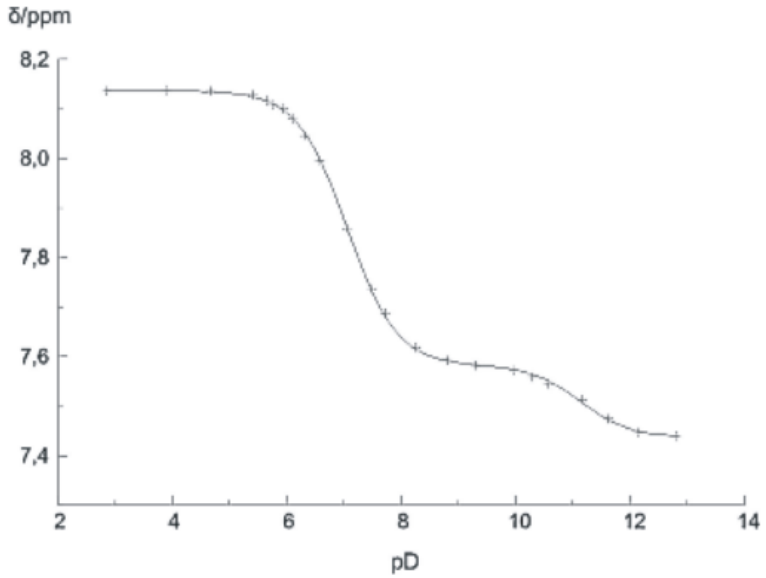

Figure S2

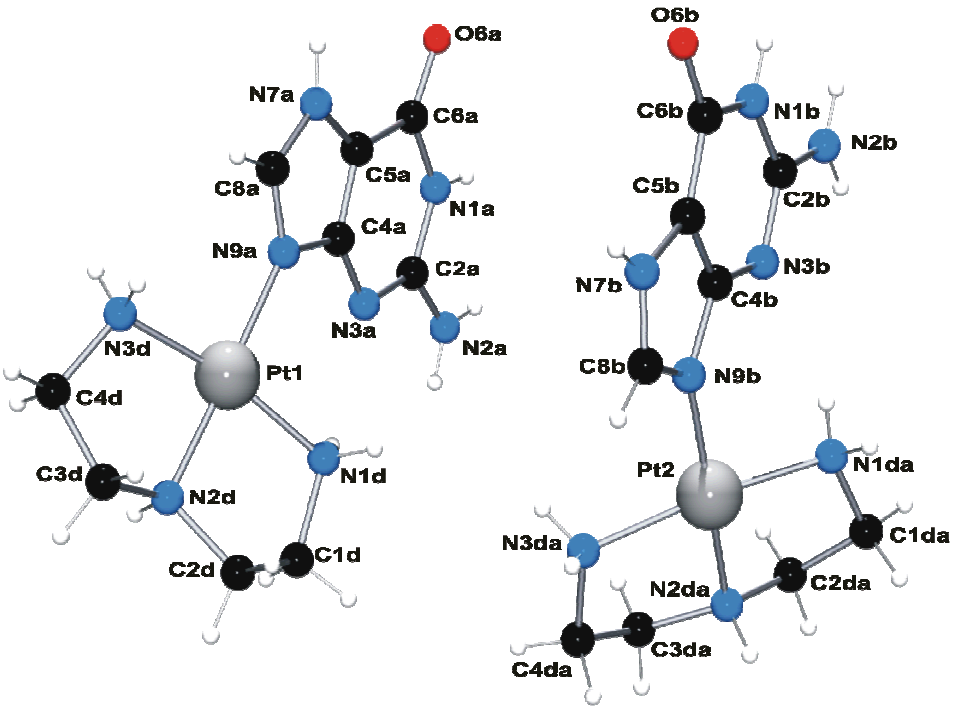

Figure S3

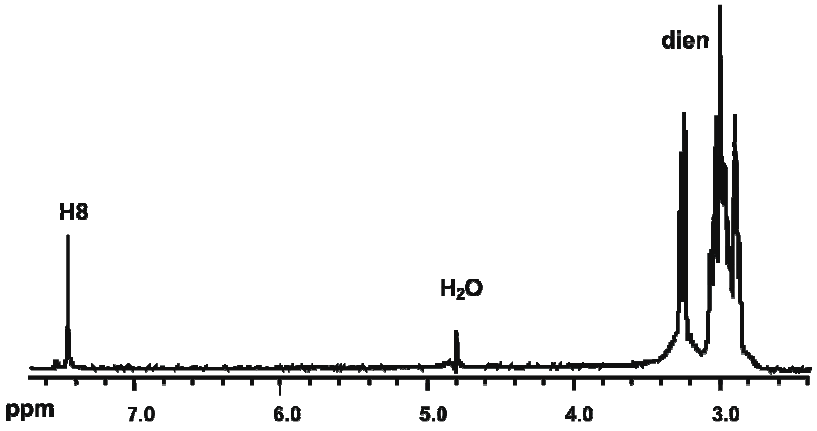

Figure S4

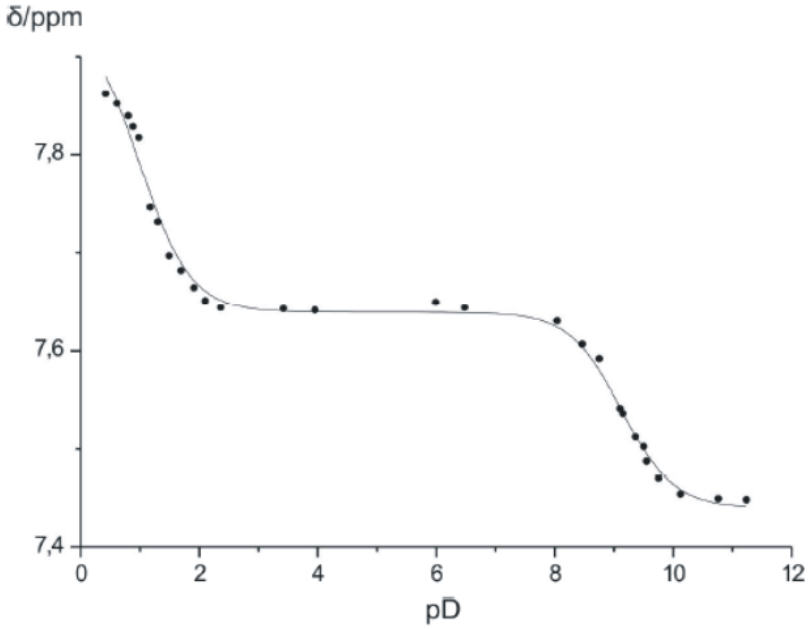

Figure S5

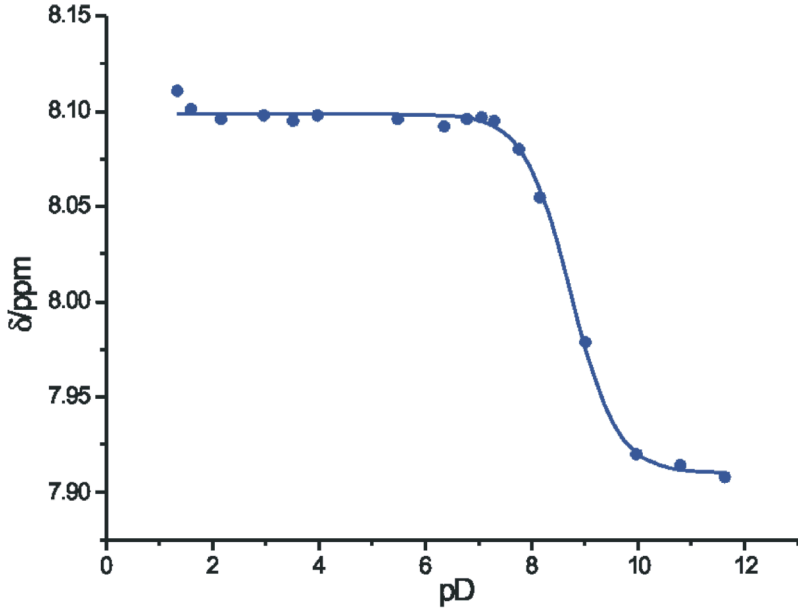

Figure S6

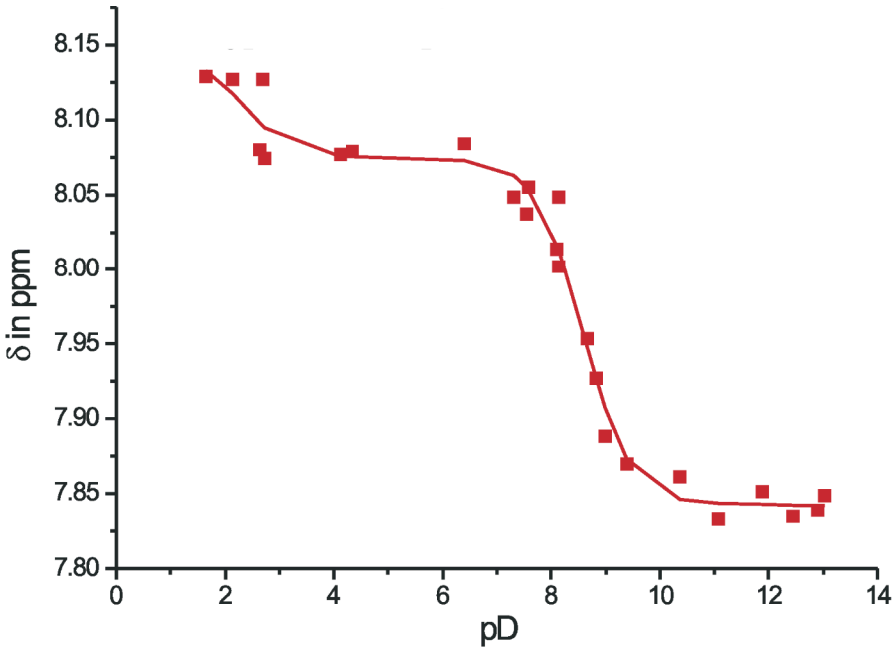

Figure S7

Table S1

Complex: $[Pt(dien)(GH_2\text{-}N7)]^{2+}$

Method: B3LYP

Basis set: GEN

Target: FREQ

Charge: 2+ (212 e-)

Multiplicity: 1

Stoichiometry: $C_9H_{18}N_8OPt$ (37 atoms)

Energy minimum: 3 / 3 (-985.800931 Hartree = -2588220.3088 kJ/mol)

Temperature: 298.15 Kelvin

Pressure: 1.000000 Atm

Eo: -2587392.507 kJ/mol (Eo = Eelec + ZPE)

E: -2587346.288 kJ/mol (E = Eo + Evib + Erot + Etrans)

H: -2587343.809 kJ/mol (H = E + R*T)

G: -2587512.369 kJ/mol (G = H - T*S)

E thermal: 874.021 kJ/mol

Cv: 291.533 J/(mol*K)

S: 565.350 J/(mol*K)

Basis func: 310 / 620

N	-2.50461	-2.19028	-0.93683
C	-3.08277	-1.06126	-0.39335
C	-2.01808	-0.21274	-0.08704
N	-0.81977	-0.84408	-0.42788
C	-1.15735	-2.02101	-0.9398
C	-2.31093	1.08791	0.43807
N	-3.6938	1.24579	0.64204
C	-4.67232	0.31772	0.33075
N	-4.38781	-0.86011	-0.21217
O	-1.53936	2.01987	0.68906
N	-5.94841	0.63521	0.58436
Pt	1.09491	-0.13672	-0.055

N	1.92629	-1.91754	0.74404
C	3.31616	-1.59928	1.25576
C	3.9417	-0.50508	0.3914
N	2.9669	0.63249	0.34967
C	3.21365	1.75324	-0.62111
C	1.95175	2.61716	-0.62788
N	0.74188	1.74766	-0.85557
H	-3.95259	2.15447	1.01733
H	-0.4719	-2.76016	-1.32611
H	4.09305	2.33496	-0.32491
H	3.40083	1.30712	-1.60156
H	1.99024	-2.63073	0.01316
H	1.37032	-2.33094	1.49656
H	3.20805	-1.25818	2.2895
H	3.93585	-2.5003	1.26113
H	2.92643	1.04264	1.28932
H	4.90198	-0.18187	0.80751
H	4.10421	-0.84529	-0.63506
H	2.01298	3.39388	-1.39497
H	1.81616	3.11167	0.33872
H	-0.09806	2.12095	-0.369
H	0.52889	1.6792	-1.85355
H	-6.66213	-0.04372	0.35274
H	-6.23711	1.50677	1.00489
H	-3.01097	-2.99878	-1.28226

Table S2

Complex: $[Pt(dien)(GH_2\text{-}N9)]^{2+}$

Method: B3LYP

Basis set: GEN

Target: FREQ

Charge: 2+ (212 e-)

Multiplicity: 1

Stoichiometry: $C_9H_{18}N_8OPt$ (37 atoms)

Energy minimum: 3 / 3 (-985.787275 Hartree = -2588184.4542 kJ/mol)

Temperature: 298.15 Kelvin

Pressure: 1.000000 Atm

Eo: -2587357.160 kJ/mol (Eo = Eelec + ZPE)

E: -2587310.402 kJ/mol (E = Eo + Evib + Erot + Etrans)

H: -2587307.924 kJ/mol (H = E + R*T)

G: -2587478.655 kJ/mol (G = H - T*S)

E thermal: 874.054 kJ/mol

Cv: 293.098 J/(mol*K)

S: 572.643 J/(mol*K)

Basis func: 310 / 620

C	-4.39113	-0.62191	-0.06202
C	-3.02605	-1.05475	-0.22757
C	-1.95767	-0.20433	-0.01518
N	-2.03491	1.10499	0.33654
C	-3.282	1.54152	0.51466
N	-4.38942	0.74726	0.33761
N	-0.78841	-0.92659	-0.24597
C	-1.16955	-2.16751	-0.59799
N	-2.504	-2.27613	-0.59242
Pt	1.11552	-0.163	-0.02245
N	0.57807	1.68224	-0.80971
C	1.72345	2.64295	-0.62232

C	3.04709	1.88001	-0.72558
N	2.96543	0.72507	0.23278
C	4.01057	-0.34703	0.15989
C	3.53855	-1.49113	1.05785
N	2.12584	-1.88806	0.67823
N	-3.4908	2.82513	0.86503
O	-5.41112	-1.25584	-0.21249
H	-2.69878	3.38961	1.13552
H	-4.40886	3.1808	1.09229
H	-0.50726	-2.97558	-0.86814
H	-5.31962	1.12955	0.48674
H	3.8963	2.52696	-0.48183
H	3.19549	1.47091	-1.72872
H	2.1616	-2.58885	-0.06667
H	1.67291	-2.34199	1.47535
H	3.51275	-1.17366	2.1044
H	4.2082	-2.3524	0.98338
H	2.98512	1.11199	1.18263
H	4.98362	0.03054	0.49215
H	4.09704	-0.66141	-0.88387
H	1.67582	3.44539	-1.36388
H	1.61476	3.09254	0.36931
H	-0.29986	1.98225	-0.35301
H	0.36409	1.57171	-1.80466
H	-3.04722	-3.10192	-0.82466

Table S3

Complex: $[\{Pt(dien)\}_2(GH\text{-}N7,N9)]^{3+}$

Method: B3LYP

Basis set: GEN

Target: FREQ

Charge: 3+ (346 e-)

Multiplicity: 1

Stoichiometry: $C_{13}H_{30}N_{11}OPt_2$ (57 atoms)

Energy minimum: 2 / 2 (-1428.610513 Hartree = -3750816.8493 kJ/mol)

Temperature: 298.15 Kelvin

Pressure: 1.000000 Atm

Eo: -3749505.318 kJ/mol (Eo = Eelec + ZPE)

E: -3749433.579 kJ/mol (E = Eo + Evib + Erot + Etrans)

H: -3749431.101 kJ/mol (H = E + R*T)

G: -3749660.197 kJ/mol (G = H - T*S)

E thermal: 1383.268 kJ/mol

Cv: 444.600 J/(mol*K)

S: 768.387 J/(mol*K)

Basis func: 454 / 908

C	-1.32791	2.75743	0.12005
C	-0.64846	1.49808	0.02493
C	0.74355	1.46817	-0.01649
N	1.57521	2.5384	-0.08167
C	0.95661	3.71391	-0.05023
N	-0.41407	3.82571	0.05098
N	1.13217	0.14251	-0.00175
C	-0.02319	-0.57148	0.01664
N	-1.12113	0.19065	0.02976
Pt	3.111	-0.47	0.09514
N	3.73137	0.95052	-1.29187
C	5.23931	0.95623	-1.34776

C	5.76021	-0.4592	-1.08913
N	5.12583	-0.93154	0.18811
C	5.26191	-2.3754	0.56572
C	4.33281	-2.6097	1.75571
N	2.9376	-2.11905	1.41563
N	1.66455	4.85419	-0.12212
O	-2.52925	2.98614	0.27497
H	2.67292	4.8099	-0.09244
H	1.23992	5.76993	-0.07319
H	-0.04812	-1.65153	0.01682
H	-0.84714	4.74317	0.12051
H	6.8522	-0.46958	-1.00722
H	5.46258	-1.14801	-1.88447
H	2.41873	-2.8725	0.95821
H	2.43248	-1.90663	2.27907
H	4.67055	-2.03974	2.62621
H	4.30613	-3.66658	2.0349
H	5.5247	-0.37473	0.95215
H	6.29772	-2.61642	0.82808
H	4.97256	-2.97805	-0.29956
H	5.58507	1.33155	-2.31496
H	5.59224	1.64369	-0.57311
H	3.32909	1.85979	-1.01594
H	3.34287	0.72366	-2.21108
Pt	-3.125	-0.3519	-0.12417
N	-3.01369	-1.75731	-1.69854
N	-3.73117	0.79579	1.50258
C	-5.22763	0.68173	1.66538
C	-5.71453	-0.65682	1.10729
N	-5.14592	-0.77632	-0.28189
C	-4.08632	-2.76852	-1.37155
C	-5.40336	-2.04831	-1.06205
H	-5.54974	-0.0078	-0.82491

H	-6.06749	-2.70533	-0.49456
H	-5.92339	-1.77095	-1.98324
H	-3.19737	-1.31129	-2.60272
H	-3.25277	0.49653	2.35482
H	-3.44211	1.76878	1.29402
H	-2.11567	-2.23279	-1.80441
H	-5.50544	0.79042	2.71701
H	-5.67722	1.51377	1.11484
H	-5.34736	-1.50127	1.69614
H	-6.80883	-0.6949	1.07758
H	-4.22029	-3.47153	-2.20011
H	-3.73407	-3.32388	-0.49954