

## **Supporting Information**

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Insights into the Acid-Base Properties of Pt<sup>IV</sup>-Diazidodiam(m)inedihyroxido Complexes from Multinuclear NMR Spectroscopy

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Table S1. pH-induced  $^{14}N$  chemical shift changes for complex 1 as determined by 1D  $^{14}N\{^{1}H\}$  NMR.

Assignment	Δδ (pH 1 to pH 5)	Δδ (pH 5 to pH 10)
w, Pt <sup>IV</sup> –NNN	0.55	0.11
$x$ , $Pt^{IV}$ – $NNN$	6.32	0.28
y, Pt <sup>IV</sup> –NNN	n.d. <sup>a</sup>	n.d. <sup>a</sup>
$z$ , $Pt^{IV}$ – $NH_3$	2.15 (2.23 <sup>b</sup> )	0.06 (0.10 <sup>b</sup> )

<sup>&</sup>lt;sup>a</sup> Accurate determination of the peak shift for y was not possible due to the broadness of the signal. <sup>b</sup> Chemical shift change of the coordinated ammine as determined by  $^{15}N\{^{1}H\}$  NMR.

Table S2. pH-induced  $^{14}N$  chemical shift changes for complex 2 as determined by 1D  $^{14}N\{^{1}H\}$  NMR.

Assignment	Δδ (pH 1 to pH 5)	Δδ (pH 5 to pH 9)
w, Pt <sup>IV</sup> –NNN	1.00	0.05
$x$ , $Pt^{IV}$ – $NNN$	5.33	0.22
y, Pt <sup>IV</sup> –NNN	n.d. <sup>a</sup>	n.d. <sup>a</sup>
$z$ , $Pt^{IV}$ – $NH_3$	0.93 (1.12 <sup>b</sup> )	0.07 (0.11 <sup>b</sup> )

<sup>&</sup>lt;sup>a</sup> Accurate determination of the peak shift for y was not possible due to the broadness of the signal. <sup>b</sup> Chemical shift change of the coordinated ammine as determined by  $^{15}N\{^{1}H\}$  NMR.

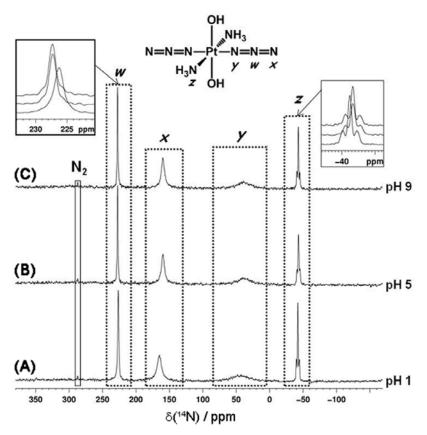


Figure S1. 1D <sup>14</sup>N{<sup>1</sup>H} NMR spectra of complex **2** in D<sub>2</sub>O in the dark at 298 K at (A) pH 1, (B) pH 5, and (C) pH 9. Assignments (internal reference N<sub>2</sub> at 287 ppm): coordinated azido ligand as labeled in structure ( $w = Pt^{IV} - NNN$ ,  $x = Pt^{IV} - NNN$ ,  $y = Pt^{IV} - NNN$ ); ammine ligand ( $z = Pt^{IV} - NH_3$ ). Inserts of signals w and z show their dependence on the pH.

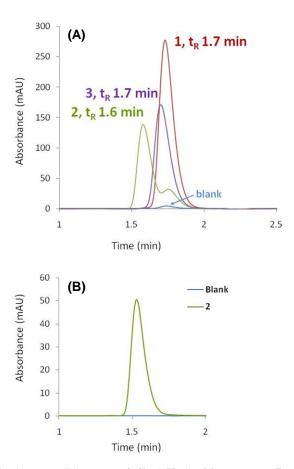


Figure S2. HPLC chromatogram in 5% water/95% acetonitrile (pH 6) with corresponding retention times at  $\lambda = 254$  nm of (A) compounds 1-3 and blank for comparison, (B) compound 2 (< 5 min after the sample was dissolved) and blank for comparison.