Supplementary Information

Formation Mechanism of 2-Methyl-2-Buten-1,4-Diol and 2-Methyl-3-Buten-1,2-Diol from 2-Methyl-1,3-Butadiene on a Head-to-Head Pivalamidato-Bridged *cis*-Diammineplatinum(III) Binuclear Complex

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Supplementary information (Figures, Equations, Schemes and The detailed discussion of the rate constants) in each section of Results and Discussion is presented under each heading.

Reactions of 1 and 7 with *p*-styrenesulfonate in acidic aqueous solutions

(eqn (S1), Scheme S1, and Figs. S1 and S2)

The expression of the conditional first-order rate constants ($k_{obs1} - k_{obs4}$)

When the mechanisms for the reactions of complex **1** and **7** with *p*-styrenesulfonate are expressed as Schemes S1 and 2, respectively, the conditional rate constants ($k_{\rm obs1}$, $k_{\rm obs2}$ and $k_{\rm obs3}$ for Schemes S1 and 2, and $k_{\rm obs4}$ for Scheme S1) are expressed as the following equations,[15]

$$k_{\rm obs1} = \frac{k_1 + \dfrac{k_1^{\#} K_{\rm h1}}{[\rm H^+]}}{1 + \dfrac{K_{\rm h1}}{[\rm H^+]}}[\rm L] + \frac{k_{-1} + \dfrac{k_{-1}^{\#} K_{\rm h2}}{[\rm H^+]}}{1 + \dfrac{K_{\rm h2}}{[\rm H^+]}} \approx \frac{k_1 + \dfrac{k_1^{\#} K_{\rm h1}}{[\rm H^+]}}{1 + \dfrac{K_{\rm h1}}{[\rm H^+]}}[\rm L] + k_{-1} + \frac{k_{-1}^{\#} K_{\rm h2}}{[\rm H^+]} \quad \text{(S1)}$$

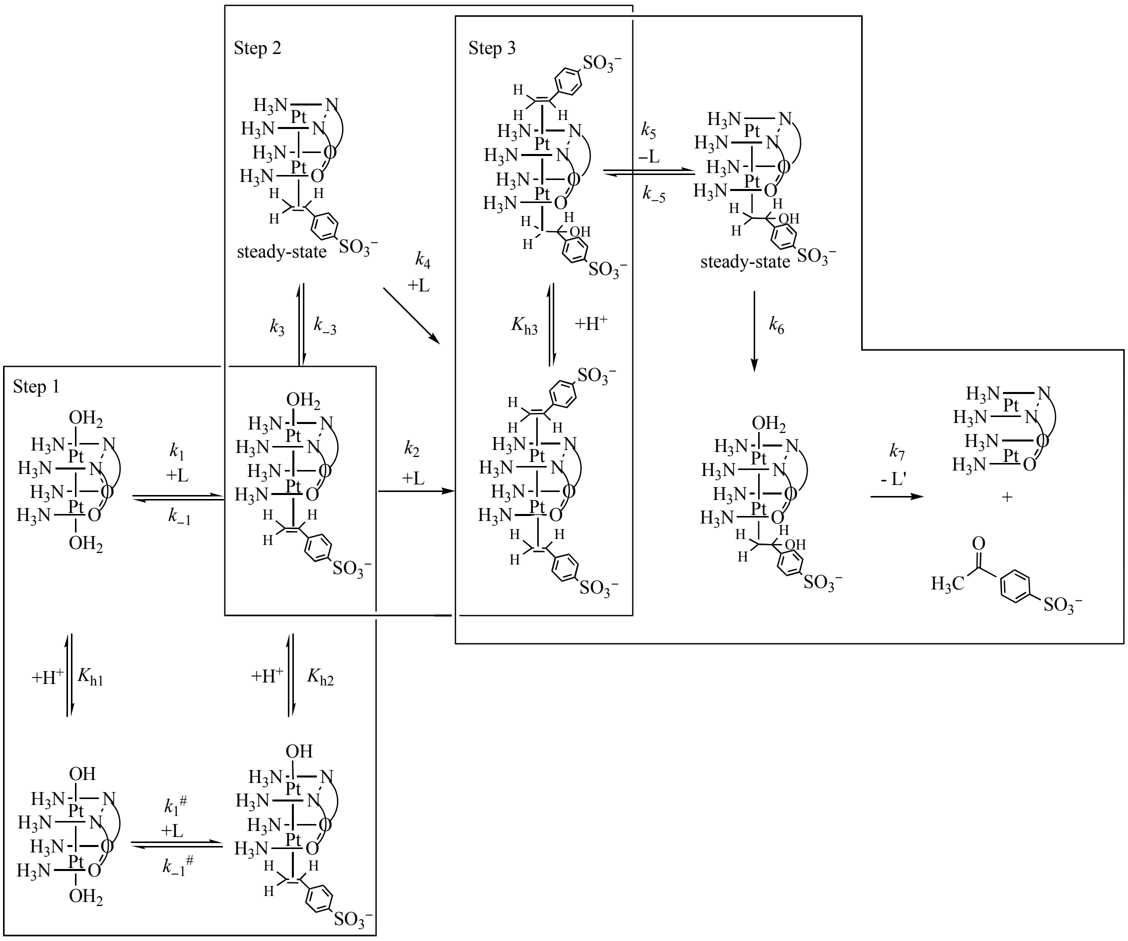
$$k_{\rm obs2} = k_2[\rm L] + \frac{k_3[\rm L]}{[\rm L] + \dfrac{k_{-3}}{k_4}} \quad \text{(S2)}$$

$$k_{\rm obs3} = \frac{\dfrac{k_5 K_{\rm h3}}{[\rm H^+] + K_{\rm h3}} + \dfrac{k_{-5} k_{-6}[\rm L]}{k_6}}{\dfrac{k_{-5}[\rm L]}{k_6} + 1} \quad \text{(S3)}$$

$$k_{\rm obs4} = k_7 \quad \text{(S4)}$$

where $C_{\rm L} \approx [\rm L]$ since $C_{\rm L} >> C_{\rm Pt}$.

Scheme S1. Reaction Mechanism for the Reaction of the HH PivalamidatoBridged Platinum(III) Dimer with Sodium *p*-Styrenesulfonate



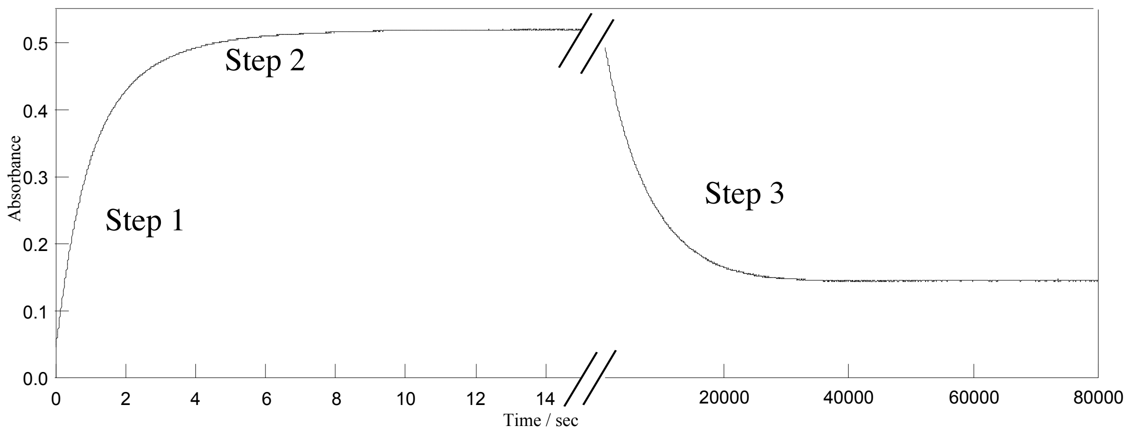


Fig. S1. The absorbance change with time at 345 nm for the reaction of the HH pivalamidato-bridged Pt(III) binuclear complex (**1**) with *p*-styrenesulfonate at $I = 2.0$ M and $T = 25°C$. ($C_{Pt} = 2.0 \times 10^{-5}$ M, $C_L = 6.0 \times 10^{-3}$ M, and $[H^+] = 0.414$ M)

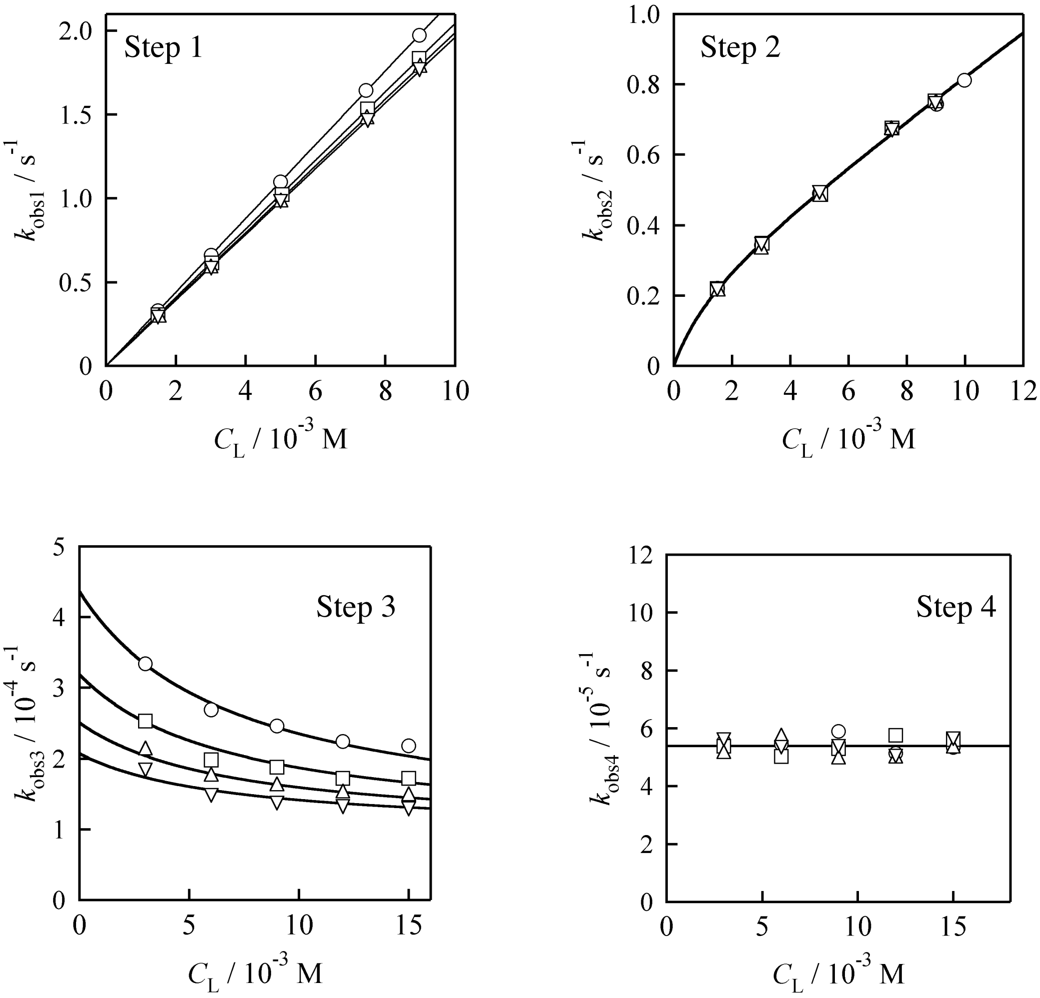


Fig. S2. Dependence of the observed rate constants (k_{obs1}, k_{obs2}, k_{obs3}, and k_{obs4}) on C_L for the reaction of the HH α-pyrrolidonato-bridged Pt(III) binuclear complex (**7**) with *p*-styrenesulfonate at I = 2.0 M, T = 25°C, and [H$^+$]/M = 0.201 (circle), 0.401 (square), 0.603 (triangle), and 0.803 (wedge).

Reactions of 1 with isoprene in acidic aqueous solutions

UV-vis spectrophotometric measurements (Figs. S3 and S4)

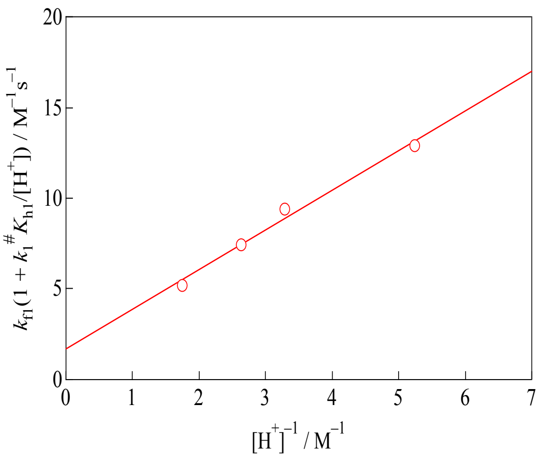


Fig. S3. The plot of $(1+K_h/[H^+])k_f$ against $[H^+]^{-1}$ for the reaction of complex **1** with 2-metyl-1,3-butadiene under various acidic conditions.

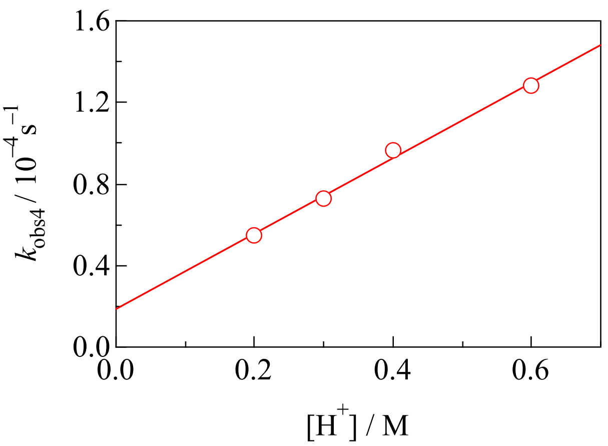


Fig. S4. Dependence of the observed rate constants k_{obs4} obtained from UV-vis spectrophotometry on $[H^+]$ for the reaction of **1** with 2-methyl-1,3-butadiene in 50% AN/50% H_2O (v/v) at 30 ºC, I = 1.0 M, and $C_{Pt} = 8.0 \times 10^{-5}$ M.

Reactions of 2 and 3 with water in acidic solutions

UV-vis spectrophotometry (Figs. S5 and S6)

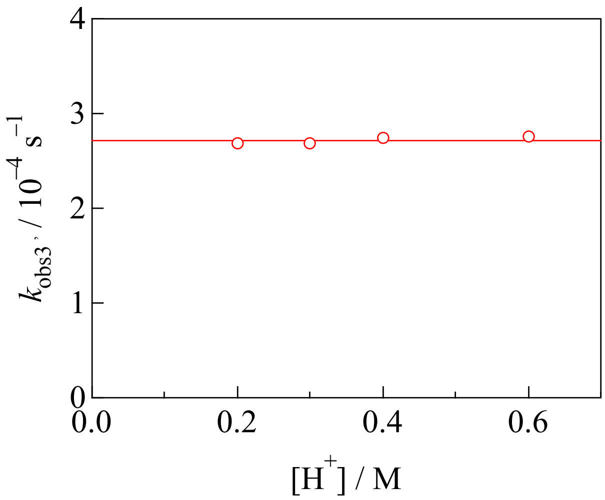


Fig. S5. Dependence of the observed rate constants $k_{obs3'}$ obtained from UV-vis spectrophotometry on [H$^+$] for the reaction of **2** and **3** with H_2O in 50% AN/50% H_2O (v/v) at 30 °C, I = 1.0 M, and C_{Pt} = 8.0 × 10^{-5} M. The initial concentration ratio of **2** to **3** was ca. 6.8:3.2.

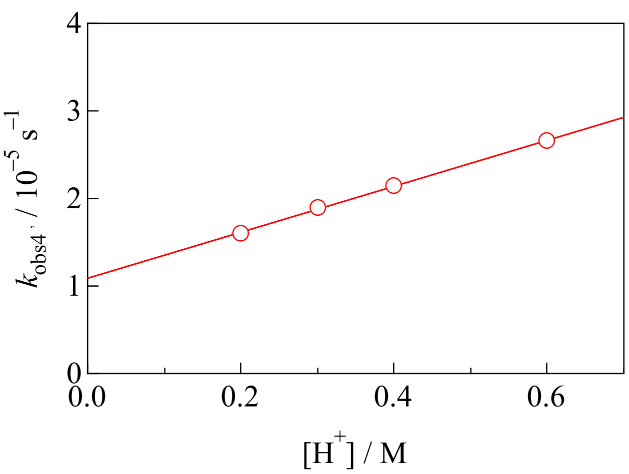


Fig. S6. Dependence of the observed rate constants $k_{obs4'}$ obtained from UV-vis spectrophotometry on [H$^+$] for the reaction of **2** and **3** with H_2O in 50% AN/50% H_2O (v/v) at 30 °C, I = 1.0 M, and C_{Pt} = 8.0 × 10^{-5} M.

[1]H NMR spectroscopy (Figs. S7–S10)

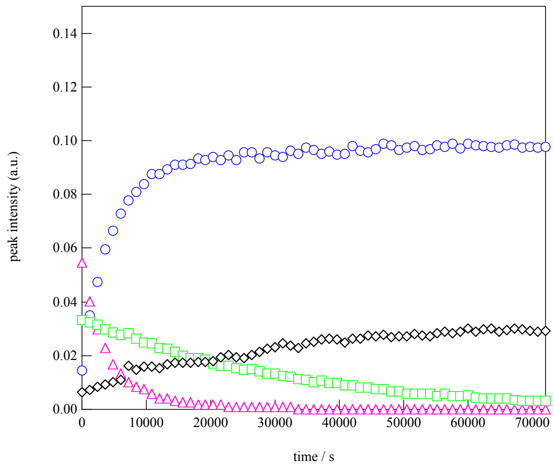


Fig. S7. Change in peak intensity of complex **2** (△), complex **3** (□), diol **4** (○) and diol **5**(◇) with time after dissolving complexes **2** and **3** into D_2O at 30ºC. The total concentration of complexes **2** and **3** is 1.5 x 10^{-3} M. The relative initial concentrations are $C_{\text{complex } \mathbf{2}} > C_{\text{complex } \mathbf{3}}$. pD = 2.89.

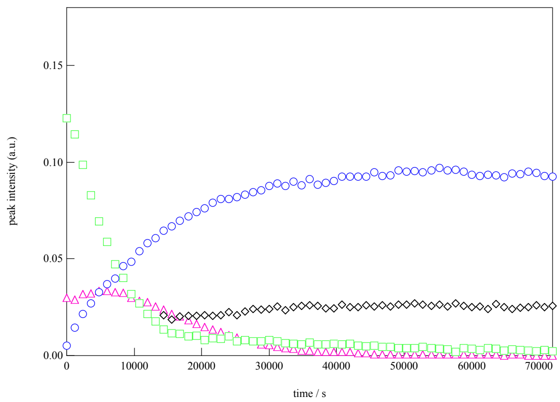


Fig. S8. Change in peak intensity of complex **2** (△), complex **3** (□), diol **4** (○) and diol **5** (◇) with time after the reaction of complex **1** with isoprene was started at 30ºC. The initial concentration of complex **1** is 1.5 x 10^{-3}M. The relative initial concentrations are $C_{\text{complex } \mathbf{2}} < C_{\text{complex } \mathbf{3}}$. pD = 2.78.

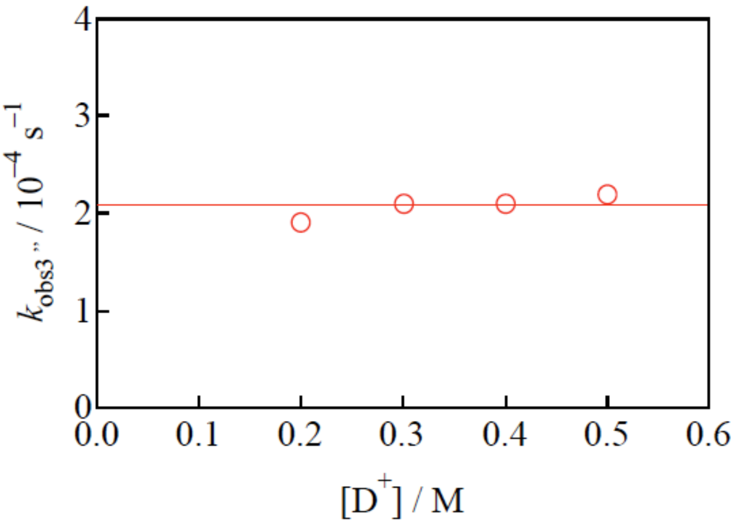


Fig. S9. Dependence of the observed rate constants $k_{obs3"}$ obtained from ^{1}H NMR spectrophotometry on [D^+] for the reaction of **2** and **3** with D_2O in 50% AN-d_3/50% D_2O (v/v) at 30 °C, C_{Pt} = 2.0 × 10^{-3} M, and I = 1.0 M.

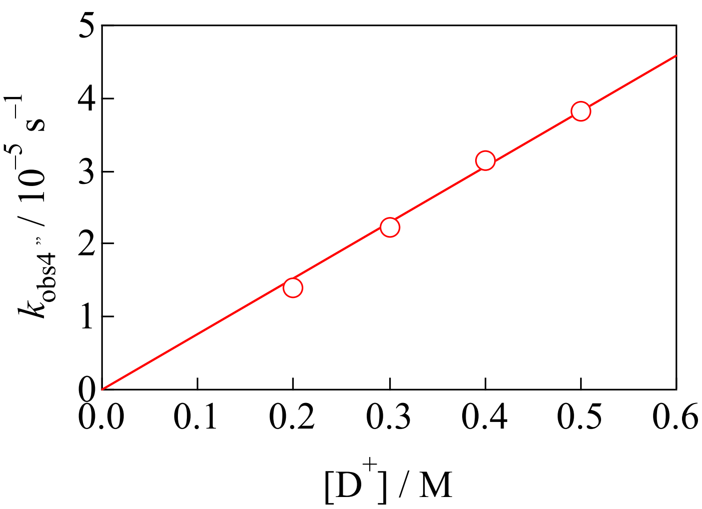


Fig. S10. Dependence of the observed rate constants $k_{obs4"}$ obtained from ^{1}H NMR spectrophotometry on [D^+] for the reaction of **2** and **3** with D_2O in 50% AN-d_3/50% D_2O (v/v) at 30 °C, C_{Pt} = 2.0 × 10^{-3} M, and I = 1.0 M.

Rate constants and mechanisms for the slow reaction steps of the reaction of 1 with isoprene

Rate constants k_{obs3}, k_{obs4}, $k_{obs3'}$, and $k_{obs4'}$ obtained by using UV-vis spectrophotometry

The detailed discussion on the rate constants k_{obs3}, k_{obs4}, $k_{obs3'}$, and $k_{obs4'}$ obtained by using UV-vis spectrophotometry

The acid-independent rate constant k_{f3} (= 2.3 × 10^{-4} s^{-1}) agrees with $k_{f3'}$ (2.7 × 10^{-4} s^{-1}) within experimental uncertainty, and these rate constants are reasonably consistent with the acid-independent rate constant $k_{r3''}$ (= k_8 = 1.8 × 10^{-4} s^{-1}), taking into account the isotope effect;[30] the attacking molecules in the process involving k_8 are H_2O and D_2O in the UV-vis and ^{1}H NMR measurements, respectively, i.e., $k_{f3} = k_{f3'} = k_{r3''} = k_8$. In the spectrophotometric and ^{1}H NMR measurements, the acid-dependent paths (k_7 and k_{-7}) could not be detected because σ-complexes **2** and **3** are in fast equilibrium, which will be discussed later.

On the other hand, both k_{obs4} and $k_{obs4'}$ involve an acid-dependent term ($k_{f4}[H^+]$ and $k_{f4'}[H^+]$) and an acid-independent term (k_{r4} and $k_{r4'}$), whereas $k_{obs4''}$ involves only an acid-dependent term ($k_{f4''}[D^+]$). k_{f4} (= 1.9 × 10^{-4} $M^{-1}s^{-1}$) is greater than $k_{f4'}$ (2.6 × 10^{-5} $M^{-1}s^{-1}$), and k_{r4} (= 1.9 × 10^{-5} s^{-1}) is significantly greater than $k_{r4'}$ (= 1.1 × 10^{-5} s^{-1}). In addition, $k_{f4'}$ is smaller than $k_{f4''}$ (= 7.6 × 10^{-5} $M^{-1}s^{-1}$). All these results indicate that k_{obs4} and $k_{obs4'}$ in Table 2 correspond not to the rate constant for step 4 in Scheme 3, but, as will be mentioned below, to those for the decomposition of **6** into mononuclear complexes.

We studied in detail the mechanism for the isomerization and decomposition reactions of HH α-pyridonato-bridged bis(ethylenediamine)platinum(II) binuclear complex in acidic aqueous solutions.[31] It was found that the isomerization reaction proceeded preferentially at pH ~7 and that the decomposition reaction proceeded exclusively at pH lower than 1. The isomerization and decomposition reactions both occurred in moderately acidic aqueous solutions. Reaction intermediates in acid-base equilibrium, such as complexes **8'** and **9'** in Scheme S2a in which one of the oxygen atoms in the bridging ligands is dissociated, were postulated for both the isomerization and decomposition reaction mechanisms in order to explain these experimental results.[31]

It is well known that olefins easily coordinate to Pt(II) ions.[32] Thus, in the presence of excess isoprene, the aqua ligands in **8'** and **9'** in Scheme S2a would be replaced almost completely by isoprene (**8** and **9** in Scheme S2b) since k_{obs4} did not depend on C_L (Fig. 7). Coordination of isoprene to **8'** and **9'** accelerates the decomposition of the dimer, explaining why $k_{f4'} < k_{f4}$ and $k_{r4'} < k_{r4}$. In Scheme S2, in the absence of isoprene (a) and in the presence of isoprene (b), $k_{obs4'}$ and k_{obs4} consist of acid-independent and acid-dependent terms, as shown in eqs 18 and 19, respectively. Thus $k'_{f4} = k'_{12}$, $k'_{r4} = k'_{11}$, $k_{f4} = k_{12}$, and $k_{r4} = k_{11}$.

$$k_{obs4'} = k'_{11} + k'_{12}[H^+] \qquad (18)$$

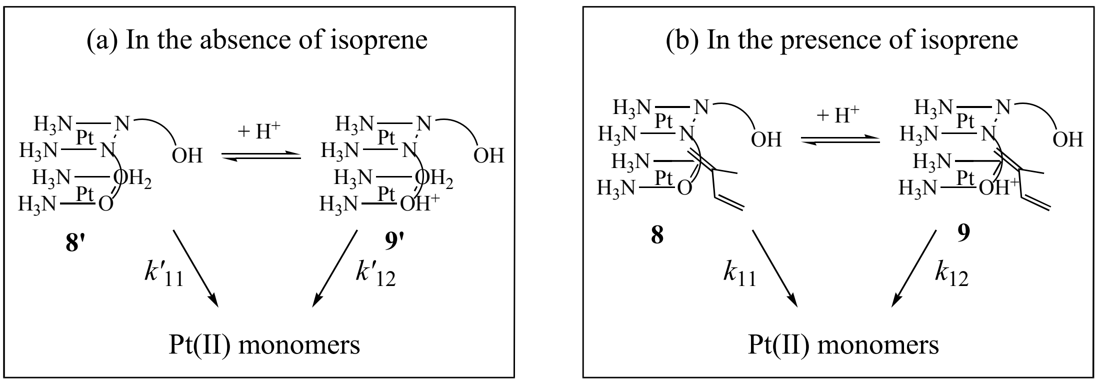
$$k_{obs4} = k_{11} + k_{12}[H^+] \qquad (19)$$

References

30 H. Fukushima, H. Mori, M. Arime, S. Iwatsuki, K. Ishihara and K. Matsumoto, *Eur. J. Inorg. Chem.*, 2011, 1930-1936.

31 To be published elsewhere.

32 R. H. Crabtree, "The Organometallic Chemistry of the Transition Metals", 3rd ed., John Wiley & Sons, New York, 2001.



Scheme S2. Reaction Mechanism for the Decomposition of the HH Pivalamidato-Bridged Platinum(II) Binuclear Complex in the absence (a) and the presence (b) of isoprene in acidic solution

Table S1. Rate constants (k_{obs1}) determined by monitoring the absorbance change at 334 nm with time for the reaction of the HH pivalamidato-bridged *cis*-diammineplatinum(III) dimer (complex **1**) with isoprene (L) in 50% AN / 50% H_2O (v/v) at 25ºC, I = 1.0 M, and C_{Pt} = 4.0 x 10^{-5}.

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs} / 10^{-2} s^{-1}		
0.191	1.62	2.49	2.59	2.34
	3.23	3.98	4.12	4.13
	6.45	8.48	8.57	8.11
	9.68	12.8	13.3	10.8
	19.4	23.2	24.4	26.4
0.304	1.62	1.44	1.52	1.43
	3.23	3.22	3.14	3.09
	6.45	6.53	6.66	6.52
	9.68	9.8	11.2	9.9
	19.4	16.9	15.3	17.3
0.380	1.62	1.21	1.35	1.21
	3.23	2.88	2.69	2.66
	6.45	5.55	5.41	5.32
	9.68	7.88	7.69	8.12
	19.4	11.9	13.5	13.9
0.570	1.62	0.69	0.64	0.63
	3.23	1.92	1.75	1.80
	6.45	3.19	3.33	3.30
	9.68	5.98	5.78	5.97
	19.4	9.44	9.12	9.15

Table S2. Rate constants (k_{obs2}) determined by monitoring the absorbance change at 334 nm with time for the reaction of complex 1 with isoprene (L) in 50% AN / 50% H_2O (v/v) at 25ºC, I = 1.0 M, and C_{Pt} = 4.0 x 10^{-5}.

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs2} / 10^{-3} s^{-1}		
0.191	1.01	1.98	2.03	1.69

	2.03	2.42	2.78	2.63
	4.06	3.35	3.56	3.56
	8.12	4.75	4.89	5.00
	10.1	4.98	5.12	5.08
	20.3	6.72	6.99	7.02
	0.50	0.97	1.11	1.07
0.304	1.01	2.31	2.18	2.50
	2.03	2.69	2.99	2.93
	4.06	3.64	3.77	3.48
	8.12	4.88	4.97	5.09
	10.1	5.88	5.95	5.87
	20.3	7.52	7.56	7.57
	0.50	0.95	0.96	0.93
0.380	1.01	2.65	2.88	2.75
	2.03	3.32	3.45	3.16
	4.06	4.08	4.33	4.07
	8.12	5.61	5.88	5.61
	10.1	6.77	6.57	6.79
	20.3	7.69	7.88	8.01
	0.50	1.22	1.15	1.17
0.570	1.01	2.69	2.98	2.85
	2.03	3.31	3.48	3.26
	4.06	4.78	4.69	4.72
	8.12	4.99	4.71	4.58
	10.1	6.28	6.32	6.45
	20.3	7.98	7.78	8.09
	0.50	0.71	0.70	0.70

Table S3. Rate constants (k_{obs3} and k_{obs4}) determined by monitoring the absorbance change at 334 nm with time for the reaction of complex 1 with isoprene (L) in 50% AN / 50% H_2O (v/v) at 30ºC, I = 1.0 M, and $C_{Pt} = 8.0 \times 10^{-5}$ M.

$[H^+]$ / M	C_L / 10^{-2} M	k_{obs3} / 10^{-4} s^{-1}		k_{obs4} / 10^{-5} s^{-1}	
0.20	0.40	2.16	1.95	5.73	4.61
	0.80	2.21	2.16	5.79	5.44
	1.20	2.18	2.16	5.45	5.53
	1.60	2.24	2.18	5.89	5.42
0.30	0.40	2.16	1.89	7.35	6.44
	0.80	2.33	2.17	7.52	7.41
	1.20	2.38	2.25	7.58	7.69
	1.60	2.29	1.99	7.37	6.76
0.40	0.40	2.48		9.52	
	0.80	2.72		9.72	
	1.20	3.00		9.90	
	1.60	2.49		9.49	
0.60	0.40	2.17		12.93	
	0.80	2.44		12.54	
	1.20	2.34		12.81	
	1.60	2.21		12.98	

Table S4. Rate constants (k_{obs3} and k_{obs4}) determined by monitoring the absorbance change at 334 nm with time for the reaction of complexes 2 and 3 with H_2O in 50% AN / 50% H_2O (v/v) at 30ºC, I = 1.0 M, and C_{Pt} = 8.0 x 10^{-5} M.

$[H^+]$ / M	k_{obs3} / 10^{-4} s^{-1}	k_{obs4} / 10^{-5} s^{-1}
0.20	2.68	1.60
0.30	2.68	1.89
0.40	2.74	2.15
0.60	2.76	2.66

Table S5. Rate constants (k_{obs3} and k_{obs4}) determined by monitoring the integrated peak intensity changes of complex **2**, diol **4**, and diol **5** with time for the reactions of complexes **2** and **3** with D_2O in 50% AN-d_3 / 50% D_2O (v/v) at 30ºC and I = 1.0 M. The total concentration of complexes **2** and **3** is 2.0 x 10^{-3} M, and the initial concentration ratio of complex **2** to complex **3** is ca. 6.8 : 3.2.

$[DClO_4]$ / M	k_{obs3} / s^{1}	k_{obs4} / s^{1}
0.20	1.9 x 10^{4}	1.4 x 10^{5}
0.30	2.1 x 10^{4}	2.2 x 10^{5}
0.40	2.1 x 10^{4}	3.1 x 10^{5}
0.50	2.2 x 10^{4}	3.8 x 10^{5}

Table S6. The conditional rate constants (k_{obs1}, k_{obs2} and k_{obs3}) for the reaction of the HH pivalamidato-bridged *cis*-diammineplatinum(III) dimer with *p*-styrenesulfonate at I = 2.0 M and 25˚C.

Step 1 C_{HH} = 2.0 x 10^{-5} M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs1} / s^{-1}
0.207	0.500	0.706, 0.686, 0.707, 0.699
	1.00	1.01, 1.00, 0.999, 1.00
	1.50	1.27, 1.27, 1.28, 1.28
	2.00	1.54, 1.53, 1.54, 1.54
	4.00	2.66, 2.64, 2.61, 2.62
	6.00	3.70, 3.67, 3.68, 3.69
	8.00	4.80, 4.75, 4.75, 4.80
	10.0	5.66, 5.65, 5.72, 5.68
0.413	0.500	0.476, 0.466, 0.452, 0.457, 0.455, 0.454, 0.441, 0.451, 0.467
	1.00	0.630, 0.621, 0.635, 0.633, 0.642, 0.634, 0.636, 0.636
	2.00	0.994, 0.954, 0.949, 0.933, 0.946, 0.945, 0.947, 0.971
	4.00	1.63, 1.63, 1.64, 1.65, 1.64, 1.64, 1.63, 1.63, 1.64
	6.00	2.31, 2.34, 2.33, 2.36, 2.33, 2.33, 2.34, 2.33, 2.33
	8.00	3.04, 3.01, 3.01, 3.01, 2.96, 2.99, 2.98, 3.03, 3.01
	11.5	3.96, 4.07, 4.02, 4.06, 4.13, 4.05, 4.05, 4.06, 4.10

0.622	0.500	0.401, 0.391, 0.396, 0.393
	1.00	0.527, 0.534, 0.516, 0.532
	2.00	0.728, 0.728, 0.689, 0.691
	4.00	1.23, 1.30, 1.28, 1.30
	6.00	1.91, 1.87, 1.90, 1.94
	8.00	2.22, 2.38, 2.30, 2.23
	10.0	2.88, 2.74, 2.56, 2.69
1.24	0.500	0.243, 0.242, 0.245, 0.240
	0.750	0.313, 0.317, 0.306, 0.308
	1.00	0.364, 0.369, 0.370, 0.366, 0.356
	2.00	0.543, 0.556, 0.586, 0.561
	4.00	0.873, 0.857, 0.884, 0.875
	6.00	1.27, 1.29, 1.28, 1.31
	8.00	1.59, 1.53, 1.53, 1.55
	10.0	1.86, 1.85, 1.84, 1.82

Step2 $C_{HH} = 2.0 \times 10^{-5}$ M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs2} / s^{-1}
0.207	0.500	0.149, 0.153
	1.00	0.224, 0.202, 0.235
	1.50	0.301, 0.305, 0.312
	2.00	0.373, 0.364, 0.382
	4.00	0.623, 0.645, 0.610
	6.00	0.884, 0.861, 0.890
	8.00	1.15, 1.20, 1.18
	10.0	1.35, 1.34, 1.36
0.311	0.500	0.140, 0.129, 0.135
	1.00	0.230, 0.220, 0.225
	2.00	0.400, 0.412, 0.395
	4.00	0.650, 0.664, 0.638
	6.00	0.902, 0.935, 0.921
	8.00	1.13, 1.08, 1.13

	10.0	1.29, 1.30, 1.32
0.414	0.500	0.139, 0.142, 0.142
	1.00	0.226, 0.225, 0.226, 0.225, 0.227
	2.00	0.378, 0.364, 0.374, 0.380
	4.00	0.624, 0.615, 0.602, 0.641
	6.00	0.864, 0.846, 0.834, 0.865
	8.00	1.05, 0.990, 1.08
	11.5	1.43, 1.43, 1.45
0.622	0.500	0.120, 0.130, 0.123
	1.00	0.197, 0.202, 0.204
	2.00	0.363, 0.350, 0.372
	4.00	0.613, 0.612, 0.601
	6.00	0.870, 0.889, 0.869
	8.00	1.11, 1.16, 1.08
	10.0	1.34, 1.23, 1.38

Step3 C_{HH} = 2.0 x10^{-5} M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs3} / 10^{-5} s^{-1}
0.103	1.00	23.3
	2.00	19.5, 19.5
	4.00	16.7
	8.00	13.6
	12.0	11.5
	16.0	10.2
	20.0	9.05
0.207	1.00	21.1
	4.00	15.0
	8.00	12.1
	12.0	10.2
	16.0	9.30
	20.0	8.55
0.311	1.00	18.0

	2.00	15.7
	4.00	13.3
	8.00	9.95
	12.0	8.27
	16.0	7.62
	20.0	6.82
1.24	1.50	9.04
	2.00	7.85
	4.00	6.92
	8.00	5.57
	12.0	4.98
	16.0	4.92
	20.0	4.72

Table S7. The conditional rate constants (k_{obs1}, k_{obs2}, k_{obs3} and k_{obs4}) for the reaction of the HH α-pyrrolidonato-bridged *cis*-diammineplatinum(III) dimer with *p*-styrenesulfonate at I = 2.0 M and 25˚C.

Step 1 C_{HH} = 2.0 x 10^{-5} M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs1} / s^{-1}
0.201	1.49	0.329, 0.319, 0.331, 0.323, 0.334, 0.348, 0.320
	3.01	0.670, 0.655, 0.663, 0.680, 0.641, 0.648
	5.00	1.10, 1.09, 1.12, 1.10, 1.08, 1.09, 1.11
	7.45	1.64, 1.66, 1.64, 1.63, 1.64, 1.65, 1.64, 1.64
	8.98	1.97, 1.97, 1.97, 1.95, 1.97, 2.00
0.401	1.49	0.301, 0.324, 0.292, 0.309, 0.314, 0.316, 0.301, 0.289
	3.03	0.615, 0.630, 0.621, 0.605, 0.594, 0.619
	5.04	1.02, 0.991, 1.11, 1.00, 0.961, 1.05
	7.49	1.55, 1.55, 1.54, 1.48, 1.47, 1.60
	8.97	1.81, 1.84, 1.84, 1.84, 1.84, 1.82, 1.85
0.602	1.52	0.312, 0.316, 0.309, 0.287, 0.295, 0.309, 0.287
	3.00	0.600, 0.590, 0.580, 0.601, 0.602, 0.604

	5.01	0.997, 0.961, 0.949, 1.00, 1.01, 0.996, 1.03, 0.972
	7.47	1.52, 1.48, 1.51, 1.48, 1.45, 1.48
	9.00	1.78, 1.79, 1.74, 1.80, 1.84, 1.81
0.803	1.49	0.297, 0.319, 0.281, 0.283, 0.294, 0.288, 0.276
	3.01	0.582, 0.586, 0.595, 0.571, 0.579
	5.00	0.976, 0.974, 0.963, 1.00, 0.980, 1.01, 0.971, 0.980
	7.50	1.54, 1.40, 1.45, 1.43, 1.54, 1.45, 1.44
	8.98	1.77, 1.78, 1.72, 1.79, 1.77, 1.77

Step 2 $C_{HH} = 2.0 \times 10^{-5}$ M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs2} / s^{-1}
0.201	1.50	0.221
	3.01	0.343
	5.00	0.489
	7.49	0.675
	9.02	0.743
	9.98	0.812
0.401	1.49	0.220
	3.03	0.349
	5.04	0.487
	7.49	0.676
	8.97	0.753
0.602	1.52	0.218
	3.00	0.337
	5.01	0.487
	7.47	0.677
	9.00	0.753
0.803	1.49	0.217
	3.01	0.346
	5.00	0.493
	7.50	0.670
	8.98	0.746

Step 3 C_{HH} = 2.0 x 10^{-5} M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs3} / 10^{-4} s^{-1}
0.201	3.00	3.34
	6.00	2.69
	9.00	2.46
	12.0	2.24
	15.0	2.18
0.401	3.00	2.53
	6.00	1.98
	9.00	1.88
	12.0	1.72
	15.0	1.72
0.603	3.00	2.15
	6.00	1.78
	9.00	1.64
	12.0	1.54
	15.0	1.50
0.803	3.00	1.84
	6.00	1.48
	9.00	1.37
	12.0	1.32
	15.0	1.29

Step 4 C_{HH} = 2.0 x 10^{-5} M

$[H^+]$ / M	C_L / 10^{-3} M	k_{obs4} / 10^{-5} s^{-1}
0.201	3.00	5.54
	6.00	5.45
	9.00	5.89
	12.0	5.13
	15.0	5.33
0.401	3.00	5.38

	6.00	5.03
	9.00	5.29
	12.0	5.76
	15.0	5.61
0.603	3.00	5.19
	6.00	5.76
	9.00	5.01
	12.0	5.04
	15.0	5.38
0.803	3.00	5.61
	6.00	5.35
	9.00	5.37
	12.0	5.03
	15.0	5.64