

Supporting Information for

Unique Stepwise Substitution Reaction of a Mono(guanidinate)tetraplatinum Complex with Amidines, Giving Mono(amidinate)tetraplatinum Complexes through Mixed-ligand Intermediate Complexes

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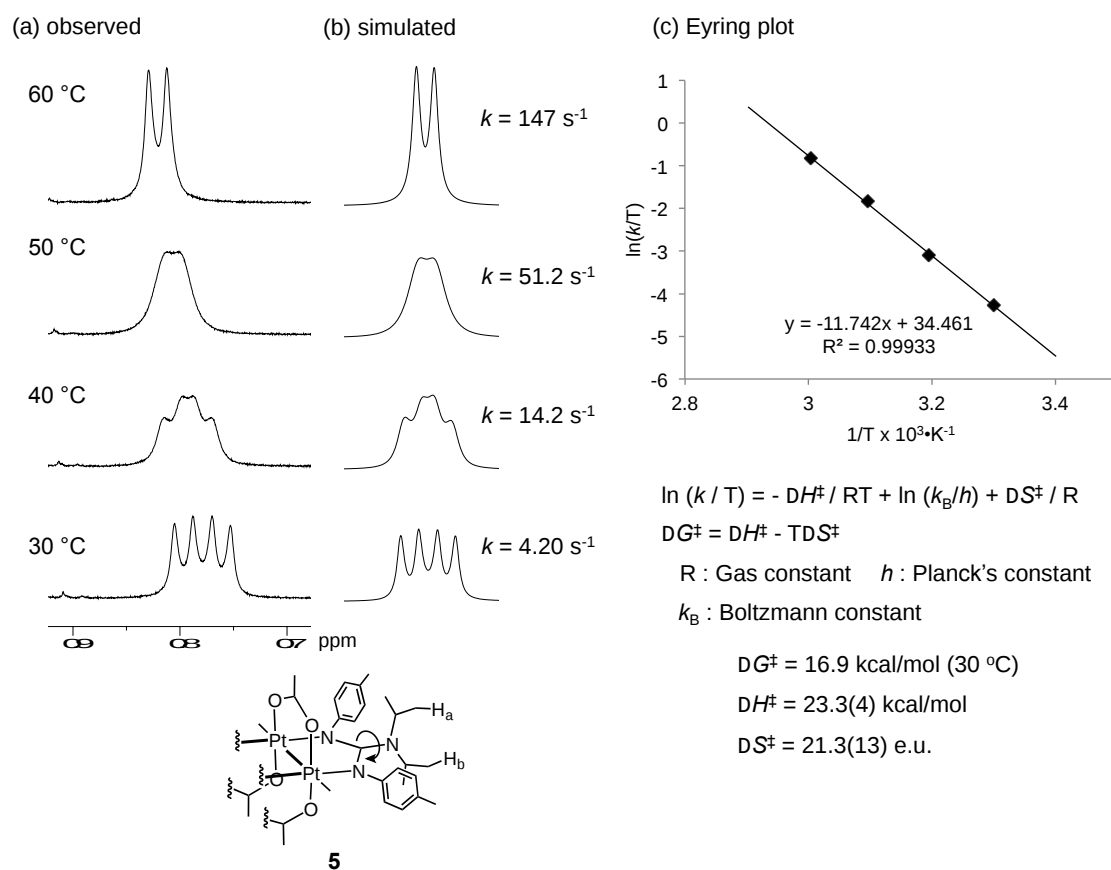


Fig S1. (a) Signals due to isopropyl groups of complex **5** observed by variable temperature ^1H NMR (400 MHz, CDCl_3) spectroscopy, (b) those of simulated spectrum, and (c) Eyring plot obtained by individual k values and temperatures.

Table S1. Crystallographic Data of **5** and **13**^{a,b}

complex	5
empirical formula	C _{36.5} H _{52.5} N ₃ O ₁₄ Pt ₄
formula weight	1537.69
temperature, K	113(1)
cryst. System	triclinic
space group	<i>P</i> -1 (#2)
<i>a</i> , Å	12.0308(6)
<i>b</i> , Å	12.3827(6)
<i>c</i> , Å	15.9563(7)
α , deg	94.2322(13)
β , deg	91.8667(13)
γ , deg	93.8168(15)
volume, Å ³	2363.64(18)
<i>Z</i>	2
calculated density, Mg m ⁻³	2.160
$2\theta_{max}$, deg	54.9
limiting indices	$-15 \leq h \leq 15, -16 \leq k \leq 16, -20 \leq l \leq 20$
absorption coefficient, mm ⁻¹	11.813
<i>F</i> (000)	1433.00
crystal size, mm	0.10 x 0.10 x 0.10
goodness-of-fit on <i>F</i> ²	1.064
reflections collected / unique	38204 / 10774 [<i>R</i> (int) = 0.0789]
no. of variables	532
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0428
<i>R</i> 1, <i>wR</i> 2 (all data)	0.0620, 0.0944
residual electron density, e Å ⁻³	2.300 (max), -2.590 (min)

^a $R1 = (\Sigma||F_o| - |F_c||) / \Sigma|F_o|$. ^b $wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma(wF_o^4)]^{1/2}$; The function minimized: $w(F_o^2 - F_c^2)^2$.

Table S1. Crystallographic Data of 5 and 13^{a,b} (continued)

complex	13
empirical formula	C _{87.64} H _{111.60} Cl ₉ N ₄ O _{28.66} Pt ₈
formula weight	3559.49
temperature, K	113(1)
cryst. System	triclinic
space group	<i>P</i> -1 (#2)
<i>a</i> , Å	12.3807(7)
<i>b</i> , Å	15.6662(9)
<i>c</i> , Å	18.7973(11)
α , deg	64.852(2)
β , deg	80.337(2)
γ , deg	82.213(2)
volume, Å ³	3245.0(4)
<i>Z</i>	1
calculated density, Mg m ⁻³	1.821
$2\theta_{max}$, deg	54.9
limiting indices	$-16 \leq h \leq 15, -20 \leq k \leq 20, -24 \leq l \leq 24$
absorption coefficient, mm ⁻¹	8.732
<i>F</i> (000)	1586.00
crystal size, mm	0.22 x 0.20 x 0.05
goodness-of-fit on <i>F</i> ²	1.067
reflections collected / unique	50725 / 14665 [<i>R</i> (int) = 0.1335]
no. of variables	647
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0863
<i>R</i> 1, <i>wR</i> 2 (all data)	0.1210, 0.2435
residual electron density, e Å ⁻³	4.22 (max), -3.65 (min)

^a $R1 = (\Sigma||F_o| - |F_c||) / \Sigma|F_o|$. ^b $wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma(wF_o^4)]^{1/2}$; The function minimized: $w(F_o^2 - F_c^2)^2$.

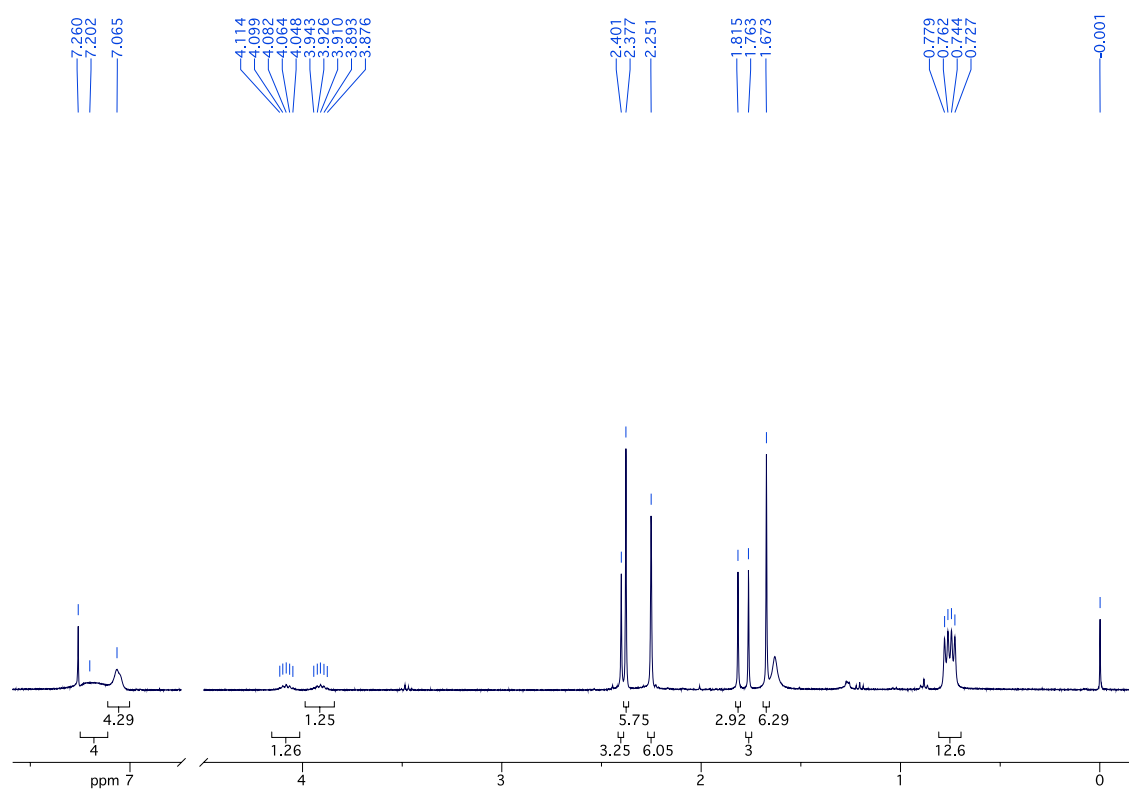


Fig S2. ¹H NMR (400 MHz, CDCl₃, 30 °C) spectrum of complex 5.

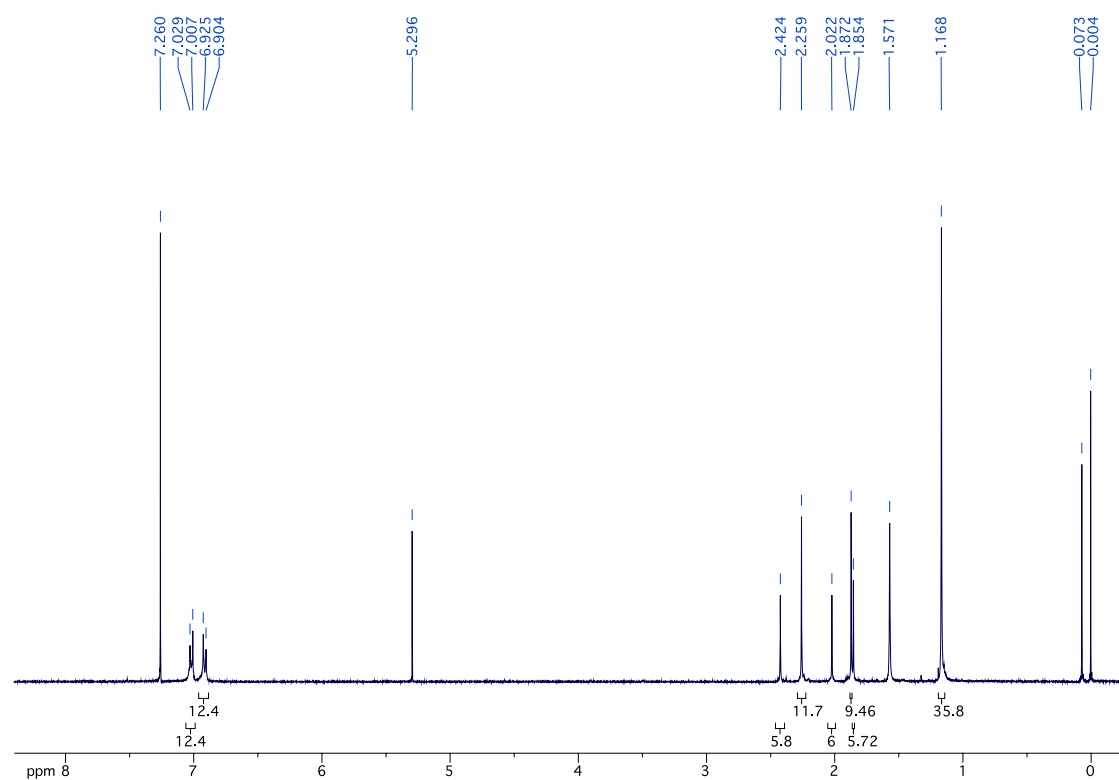


Fig S3. ¹H NMR (400 MHz, CDCl₃, 30 °C) spectrum of complex **13**.

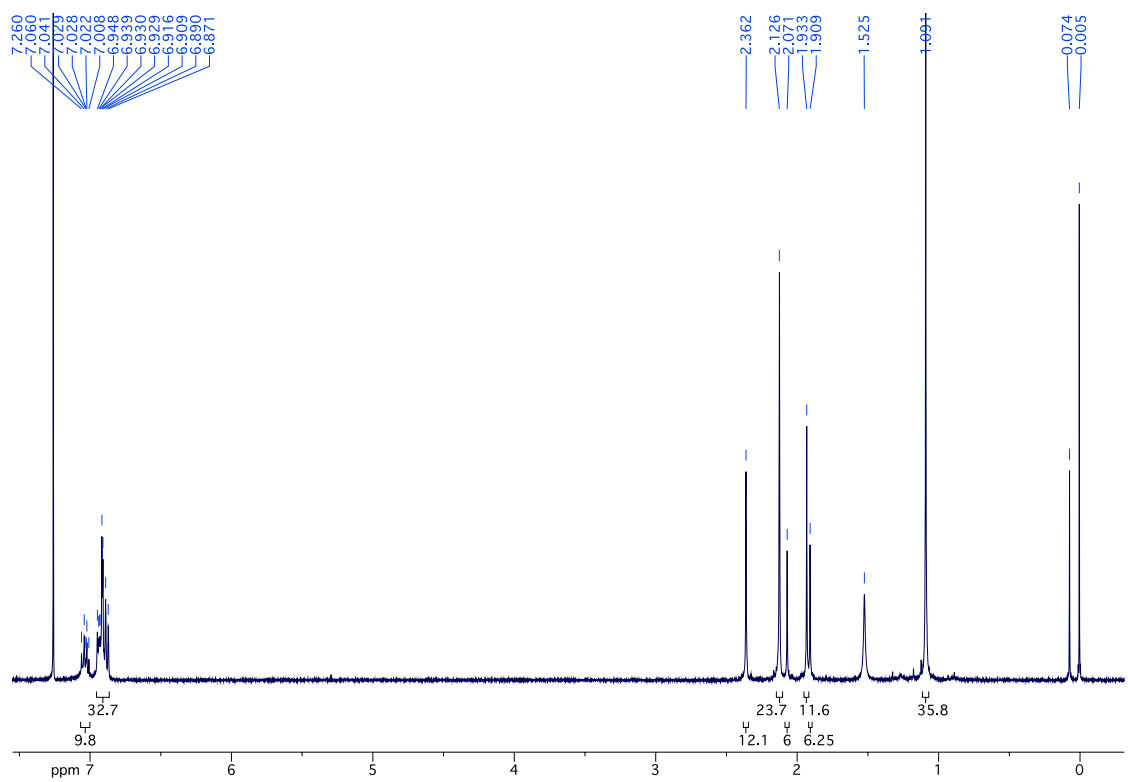


Fig S4. ¹H NMR (400 MHz, CDCl₃, 30 °C) spectrum of complex **14**.

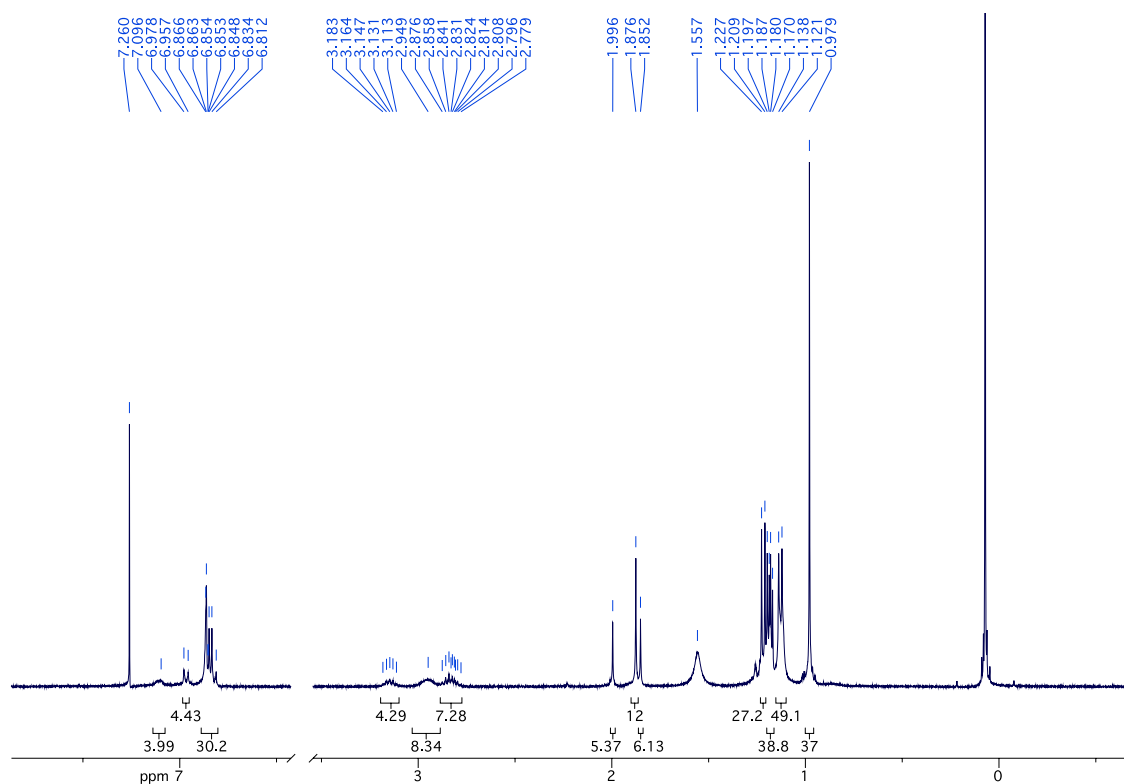


Fig S5. ^1H NMR (400 MHz, CDCl_3 , 30 °C) spectrum of complex 15.

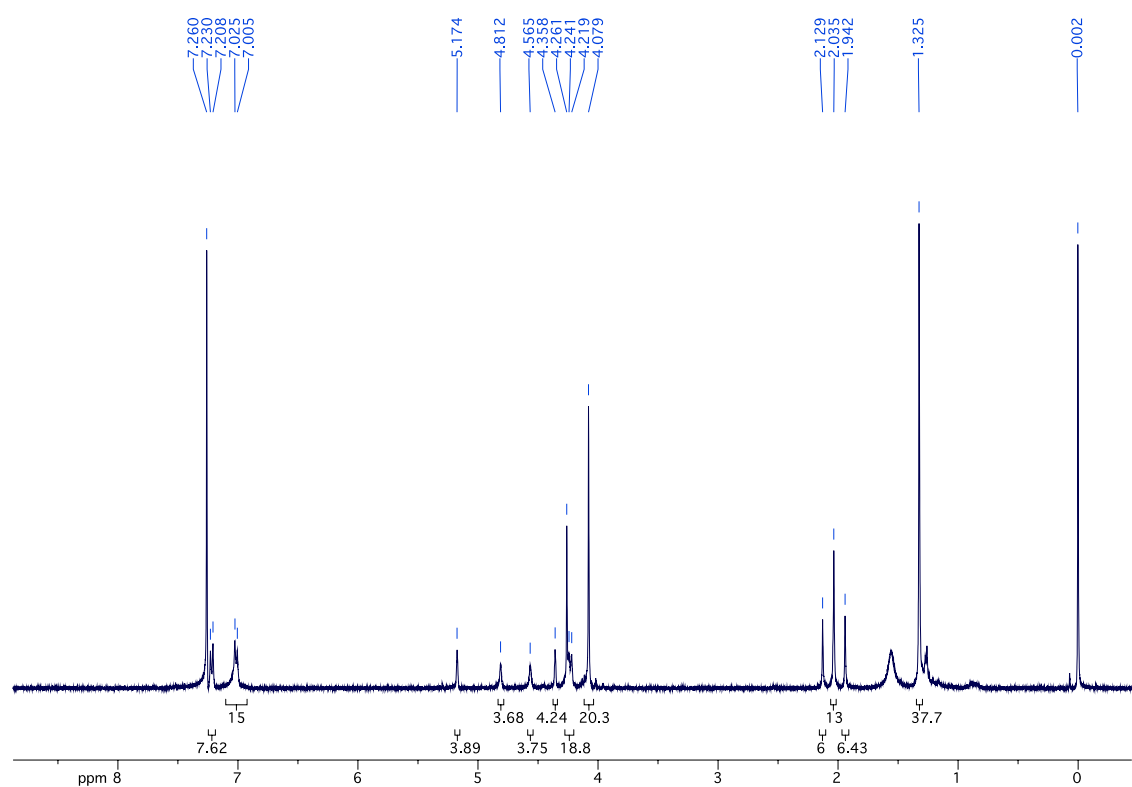


Fig S6. ^1H NMR (400 MHz, CDCl_3 , 30 $^\circ\text{C}$) spectrum of complex **16**.