Electronic Supplementary Information (ESI)

Multi-molecular emission of a cationic Pt(II) complex through hydrogen bonding interaction.

Kaho Yamaguchi,[a] Kazuma Yamawaki,[a] Takuya Kimura,[a] Junpei Kuwabara,*[a] Takeshi Yasuda,[b] Yoshinobu Nishimura,[c] and Takaki Kanbara [a]

[a] Tsukuba Research Center for Energy Materials Science (TREMS), Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki, 305-8573, Japan. E-mail: kuwabara@ims.tsukuba.ac.jp, kanbara@ims.tsukuba.ac.jp

[b] Research Center for Functional Materials, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.

[c] Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki, 305-8573, Japan.

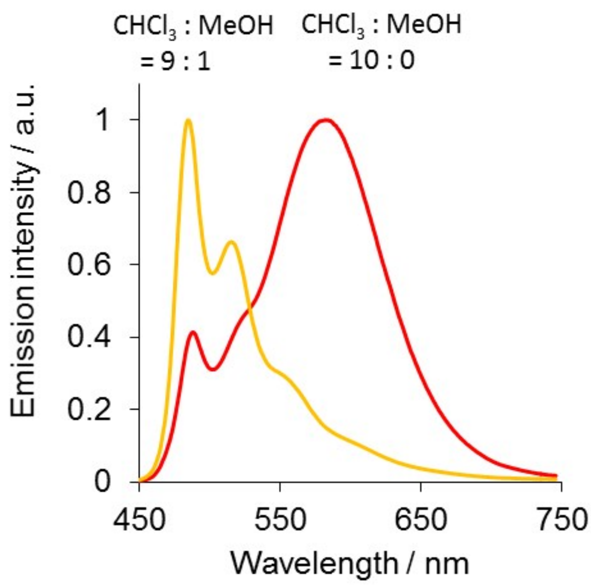


Fig. S1 Emission spectra of **Pt·Cl** in a mixture of $CHCl_3$ and methanol (10 μM).

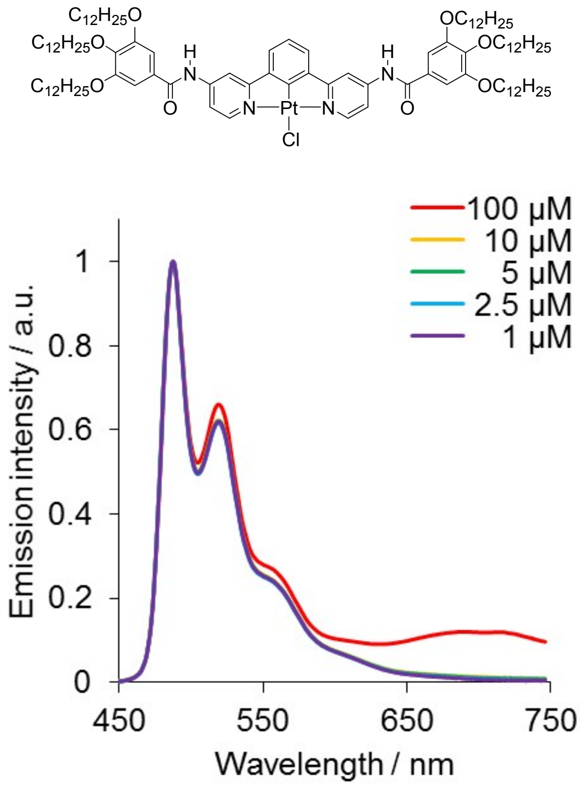
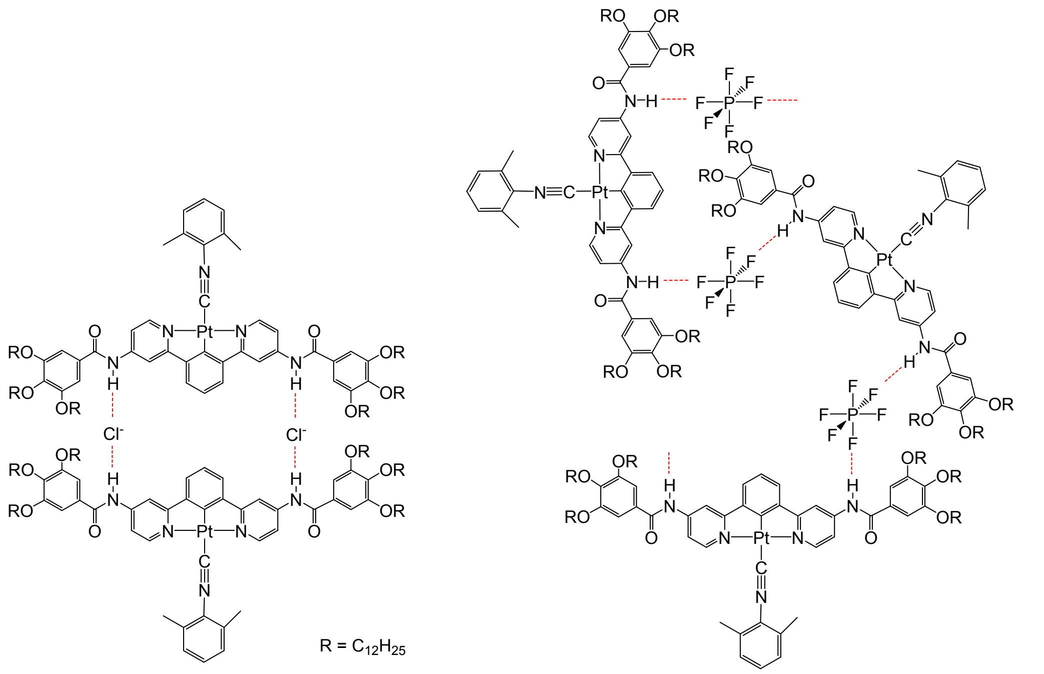


Fig. S2 Structure of the neutral Pt complex and its emission spectra at various concentration.



Pt·Cl **Pt·PF$_6$**

Fig. S3 Proposed structures with hydrogen bonding based on the ^{1}H and DOSY NMR spectra.

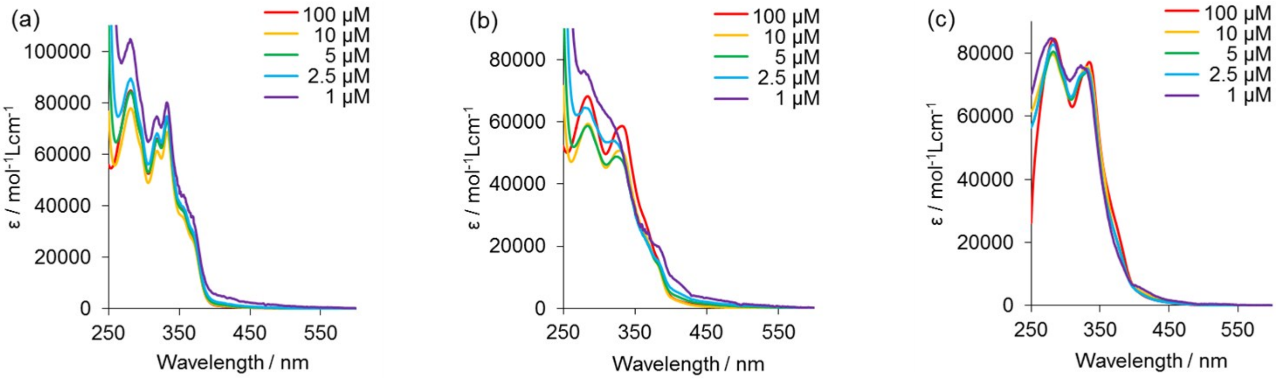


Fig. S4 Absorption spectra of (a) **Pt·B(C_6F_5)$_4$**, (b) **Pt·Cl**, and (c) **Pt·PF_6** in $CHCl_3$ at various concentrations.

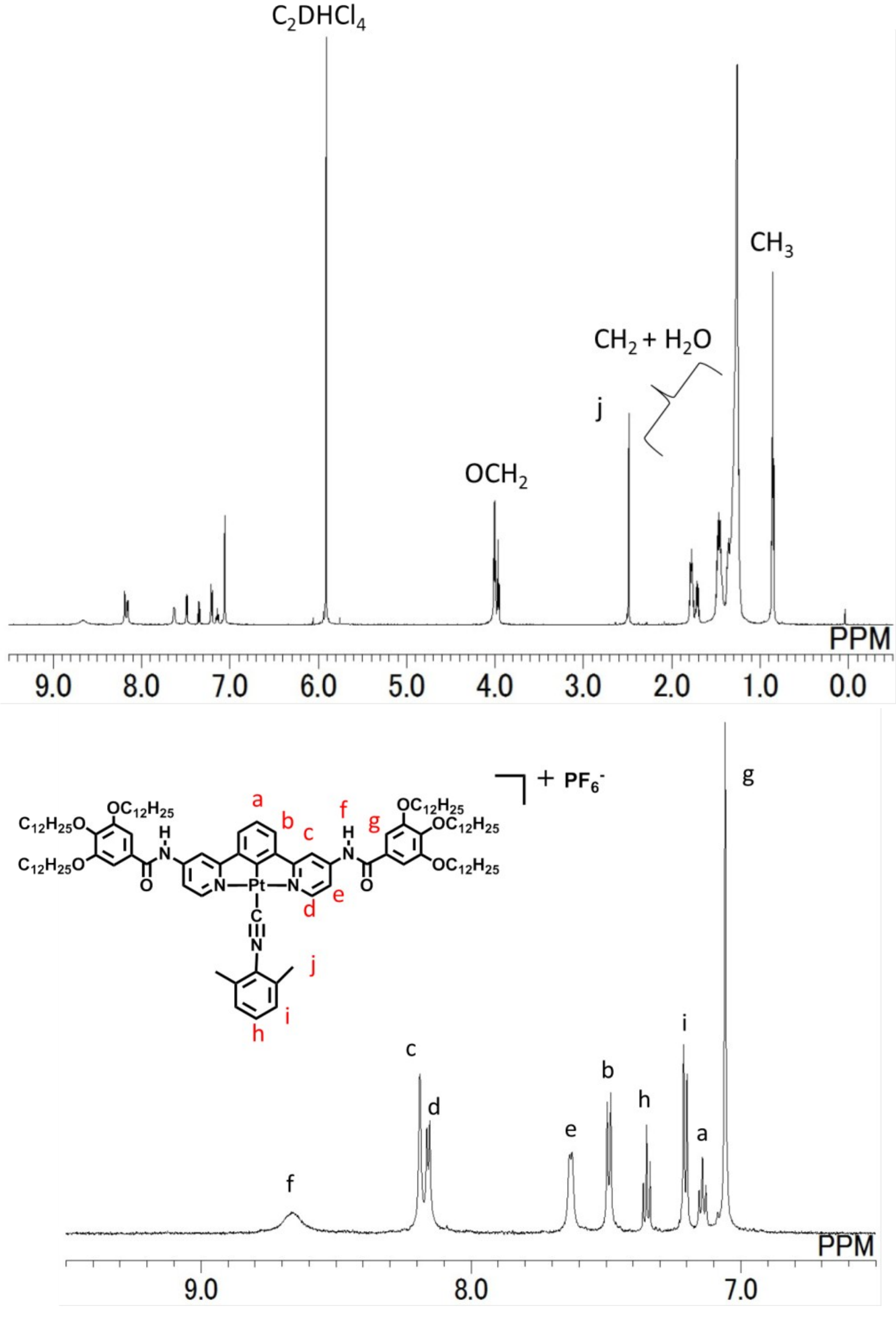


Fig. S5 ^{1}H NMR spectrum of **Pt·PF$_6$** (600 MHz, $C_2D_2Cl_4$, 4.0×10^{-3} M, 353 K).

Analysis for DOSY NMR

Einstein–Stokes equation

$$D = \frac{kT}{6\pi\eta R_H} \rightarrow R_H = \frac{6\pi}{kT} \cdot \frac{\eta}{D}$$

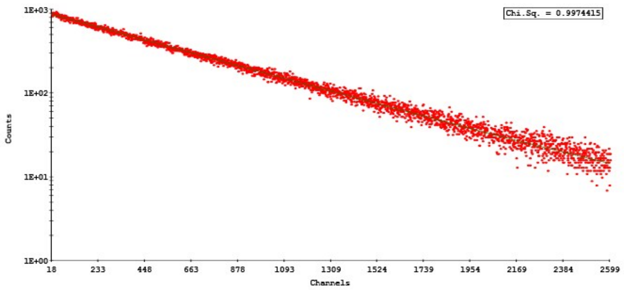
D: Diffusion constant, k: Boltzmann's constant, T: Absolute temperature, η: Viscosity of the medium, R_H: Hydrodynamic radius

Ratio of hydrodynamic radius $$\frac{R_H(\mathbf{Pt}\cdot\mathbf{Cl})}{R_H(\mathbf{Pt}\cdot\mathbf{B}(C_6F_5)_4)} = \frac{D(\mathbf{Pt}\cdot\mathbf{B}(C_6F_5)_4)}{D(\mathbf{Pt}\cdot\mathbf{Cl})} = 1.29$$

Ratio of hydrodynamic volume $$\frac{V(\mathbf{Pt}\cdot\mathbf{Cl})}{V(\mathbf{Pt}\cdot\mathbf{B}(C_6F_5)_4)} = 1.29^3 \approx 2.2$$

Analysis for kinetic traces

Pt·B(C_6F_5)$_4$



I = A+Bexp(t/τ1)

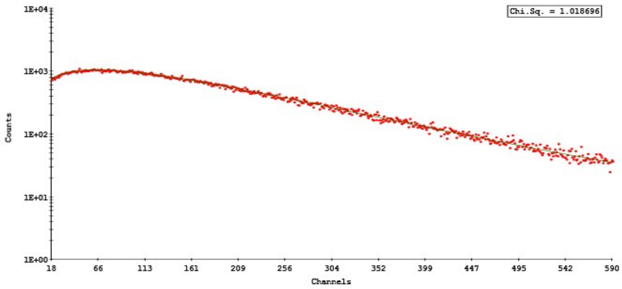
τ1 = 8.516421E-06 sec S.Dev = 2.512945E-08 sec

A = 2.141593 S.Dev = 0.1749661

B = 874.4274 S.Dev = 1.420067

CHISQ = 0.9974415 [2579 degrees of freedom]

Pt·Cl

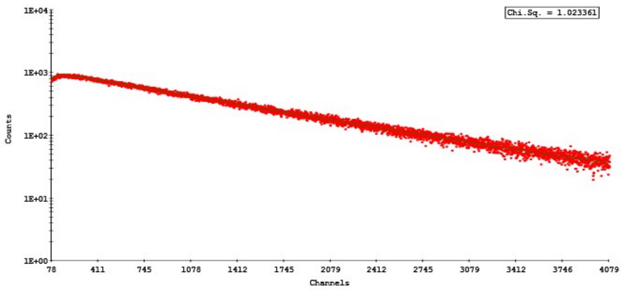


I = A+B1exp(t/τ1)+B2exp(t/τ2)

τ1 = 3.44983E-07 sec	S.Dev = 1.300902E-08 sec
τ2 = 8.948246E-07 sec	S.Dev = 6.579976E-09 sec
A = 7.643316	S.Dev = 0.627084
B1 = -1711.312	S.Dev = 12.82049
B2 = 2461.328	S.Dev = 8.43819

CHISQ = 1.018696 [568 degrees of freedom]

Pt·PF_6



I = A+B1exp(t/τ1)+B2exp(t/τ2)

τ1 = 5.019333E-08 sec	S.Dev = 2.823604E-09 sec
τ2 = 9.721266E-07 sec	S.Dev = 2.838167E-09 sec
A = 8.996995	S.Dev = 0.2226138
B1 = -247.476	S.Dev = 5.820917
B2 = 1025.245	S.Dev = 1.346489

CHISQ = 1.023361 [3997 degrees of freedom]