

Supporting Information

Coordination-based Vapochromic Behavior of a Luminescent Pt(II) Complex with Potassium Ions

Yasuhiro Shigeta,^{*a} Ryota Nanko,^b Shogo Amemori,^{a,c,d} and Motohiro Mizuno^{*a,c,d}

^a NanoMaterials Research Institute, Kanazawa University, Kanazawa 920-1192, Japan

^b College of Science and Engineering, School of Chemistry, Kanazawa University, Kanazawa 920-1192, Japan

^c Graduate School of Natural Science and Technology, Kanazawa University, Kanazawa 920-1192, Japan

^d Institute of Frontier Science Initiative, Kanazawa University, Kanazawa 920-1192, Japan

Contents

Figure S1. Crystal structures of **1·3DMA** and **1·0.75DMF** with atom labels around Pt(II) ions.

Figure S2. ¹H NMR spectrum of **1**.

Figure S3 Lattice constant refinement fitting for **1** after DMA and DMF vapor exposure.

Figure S4. Thermogravimetric analysis of DMA-vapor exposed **1**.

Figure S5. Thermogravimetric analysis of DMF-vapor exposed **1**.

Figure S6. ¹H NMR spectrum of DMA vapor exposed **1**.

Figure S7. ¹H NMR spectrum of DMF vapor exposed **1**.

Figure S8. Photographs of **1·3DMA** and **1·0.75DMF** compared with **1** in DMA and DMF solution.

Figure S9. Absorption spectra of **1** in DMA and DMF solution.

Figure S10. Photographs of **1·0.3H₂O** compared with DMF and DMA vapor exposed samples under ambient light and UV light irradiation.

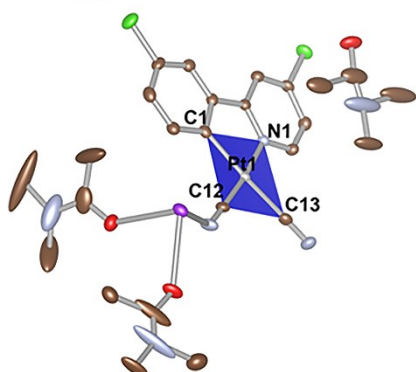
Figure S11. Emission spectrum of DMA solution of **1**.

Table S1. Selected bond length of **1·3DMA** and **1·0.75DMF** at 90 K.

Table S2. Comparison for possible molecular composition and that found from elemental analysis.

Table S3. Lattice constant refinement result for **1** after DMA and DMF vapor exposure compared with the single crystals.

1·3DMA



1·0.75DMF

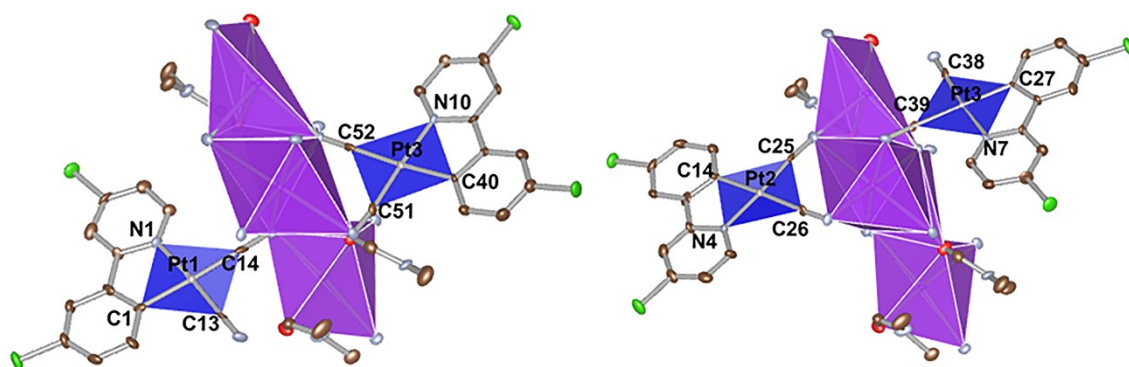


Figure S1. Crystal structures of **1·3DMA** (top) and **1·0.75DMF** (bottom) with atom labels around Pt(II) ions.

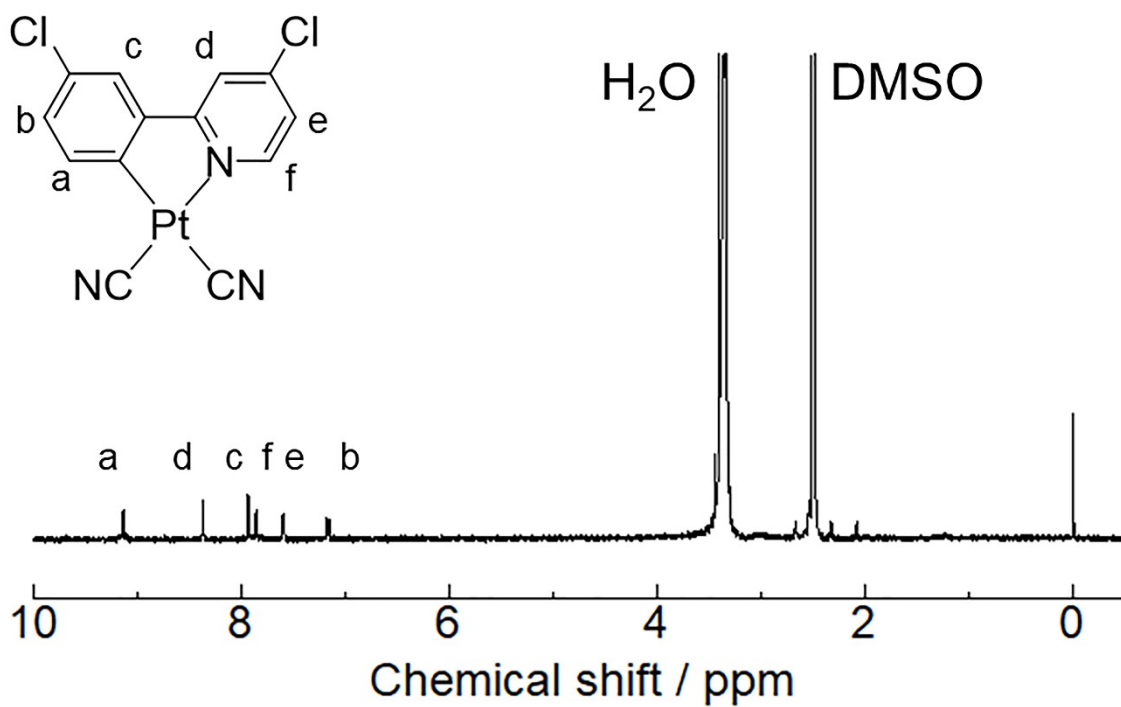


Figure S2. ^1H NMR spectrum of **1** (400 MHz, DMSO-d_6).

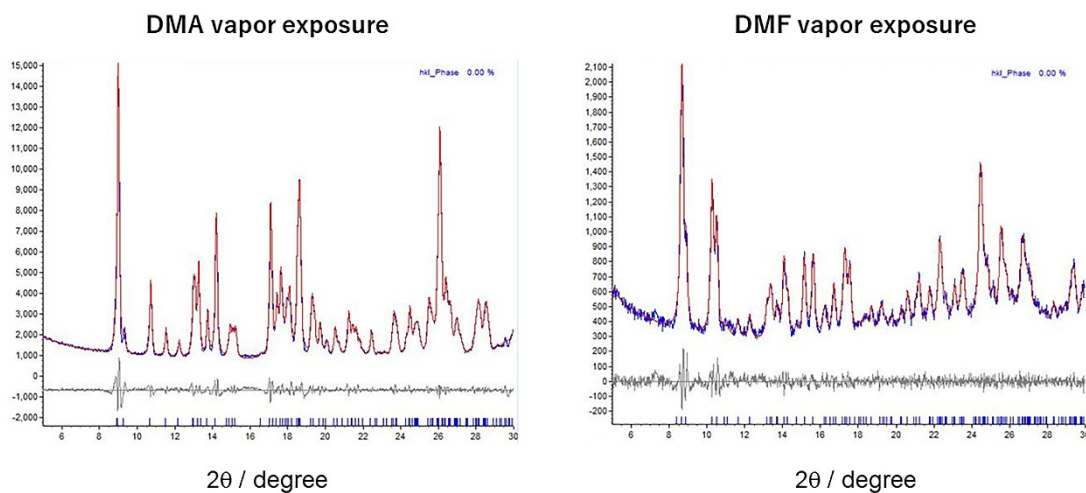


Figure S3. Lattice constant refinement fitting for **1** after DMA (left) and DMF (right) vapor exposure. Blue, red and gray lines show experimental, calculated and residual, respectively.

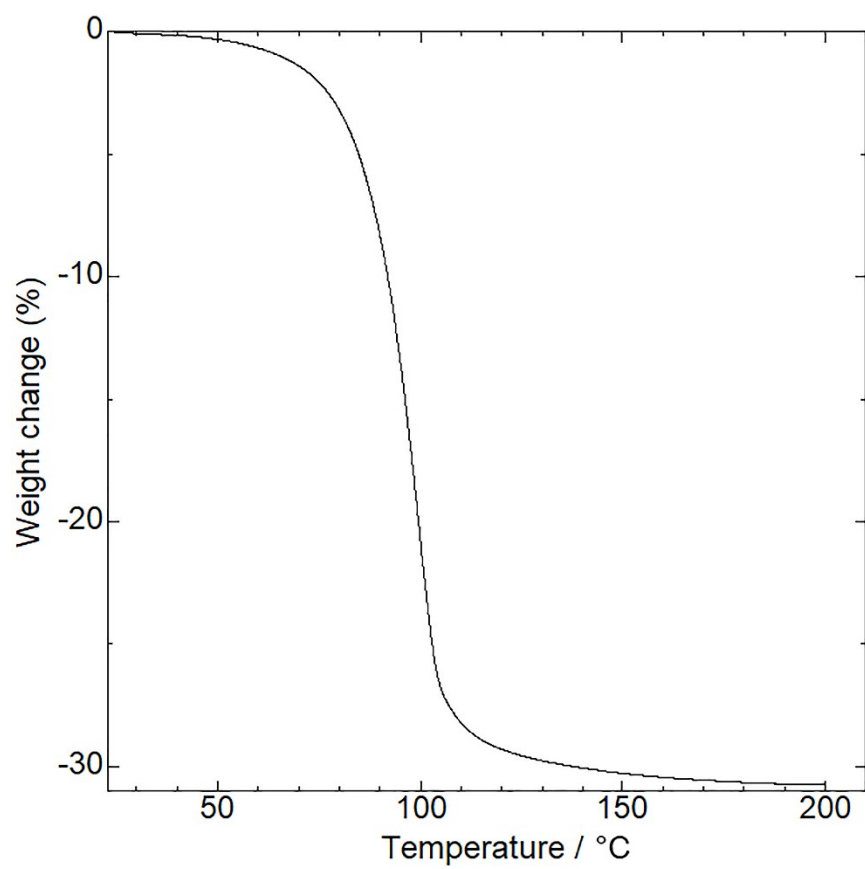


Figure S4. Thermogravimetric analysis of DMA-vapor exposed **1**.

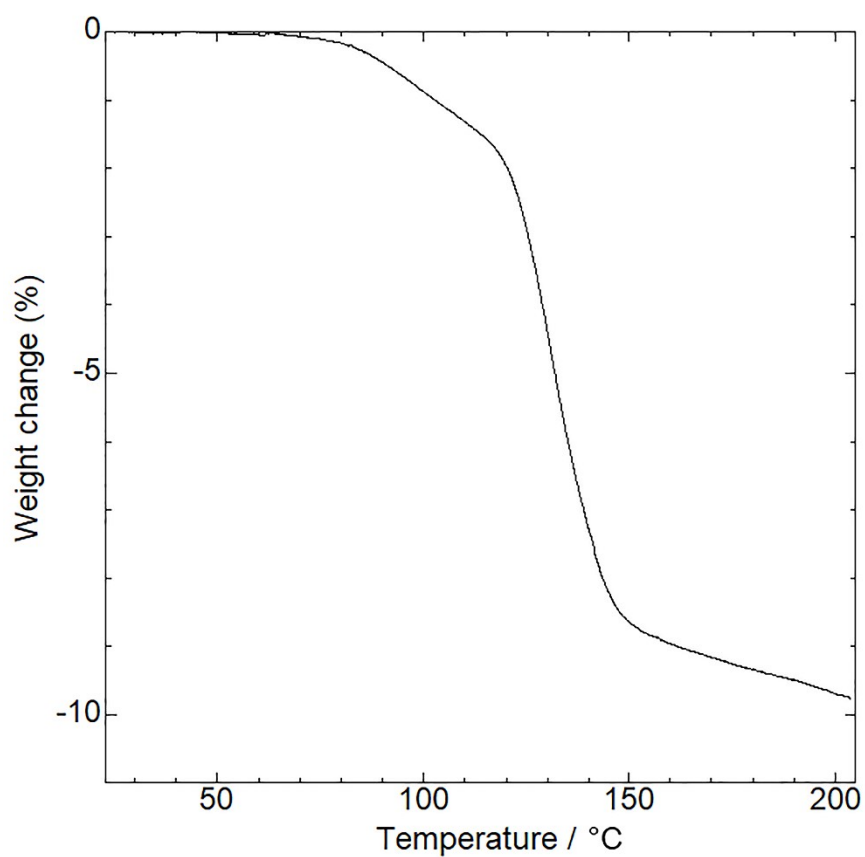


Figure S5. Thermogravimetric analysis of DMF-vapor exposed **1**.

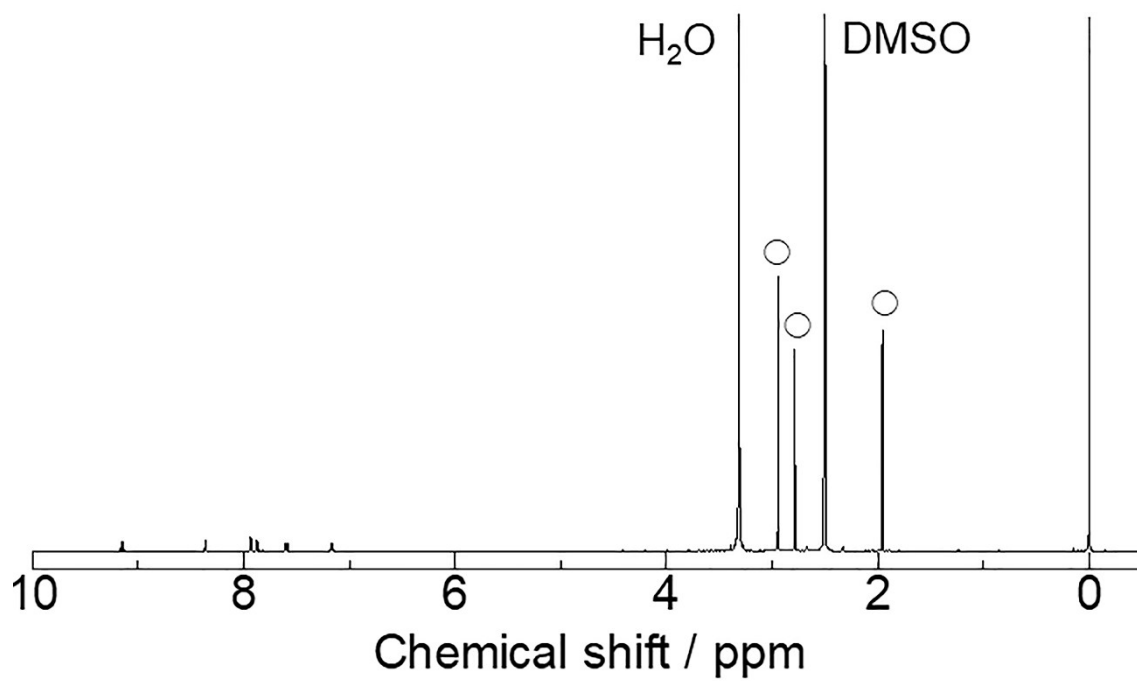


Figure S6. ^1H NMR spectrum of DMA vapor exposed **1** (400 MHz, $\text{DMSO-}d_6$). Circles indicate the signals from DMA.

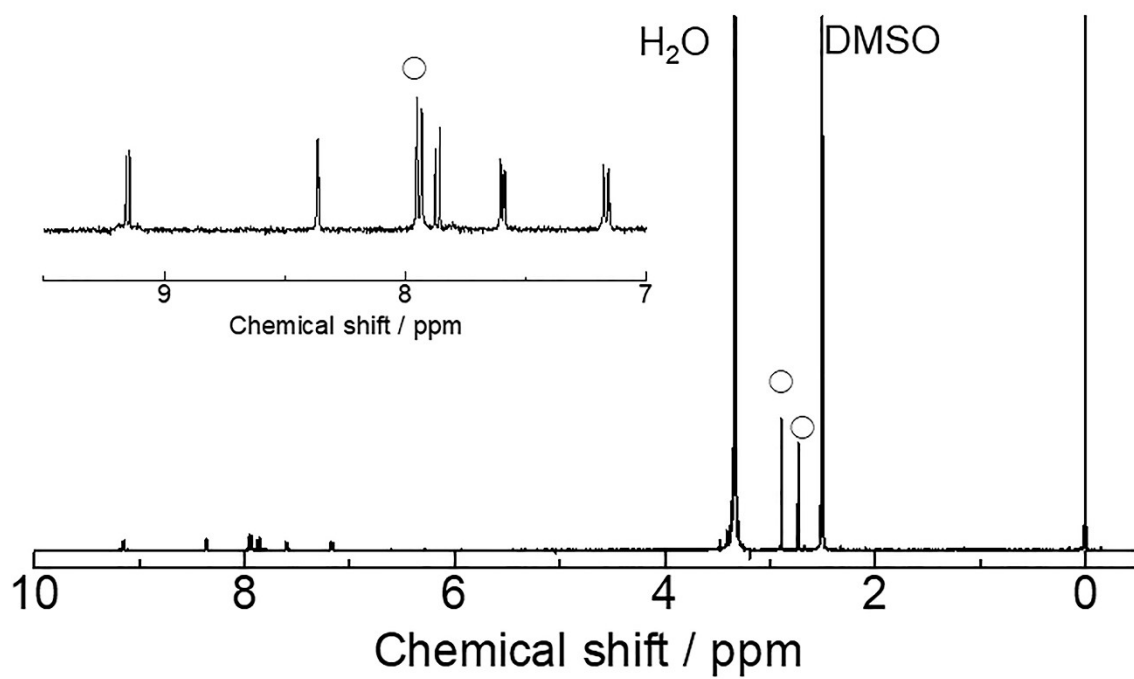


Figure S7. ^1H NMR spectrum of DMA vapor exposed 1 (400 MHz, $\text{DMSO-}d_6$). Circles indicate the signals from DMF.

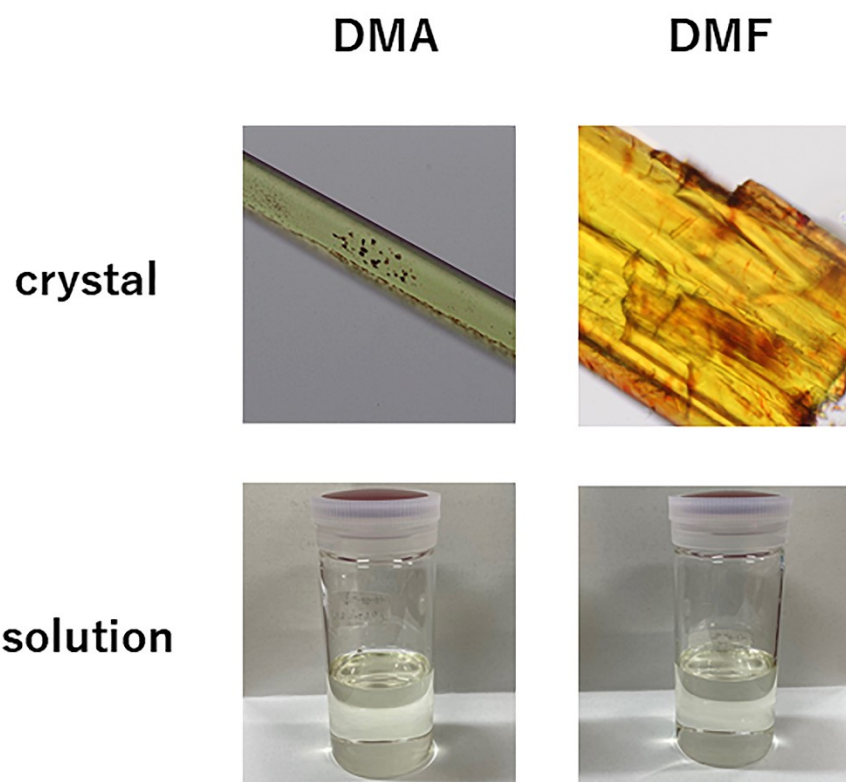


Figure S8. Photographs of $1 \cdot 3\text{DMA}$ and $1 \cdot 0.75\text{DMF}$ (top) compared with **1** in DMA and DMF solution (bottom).

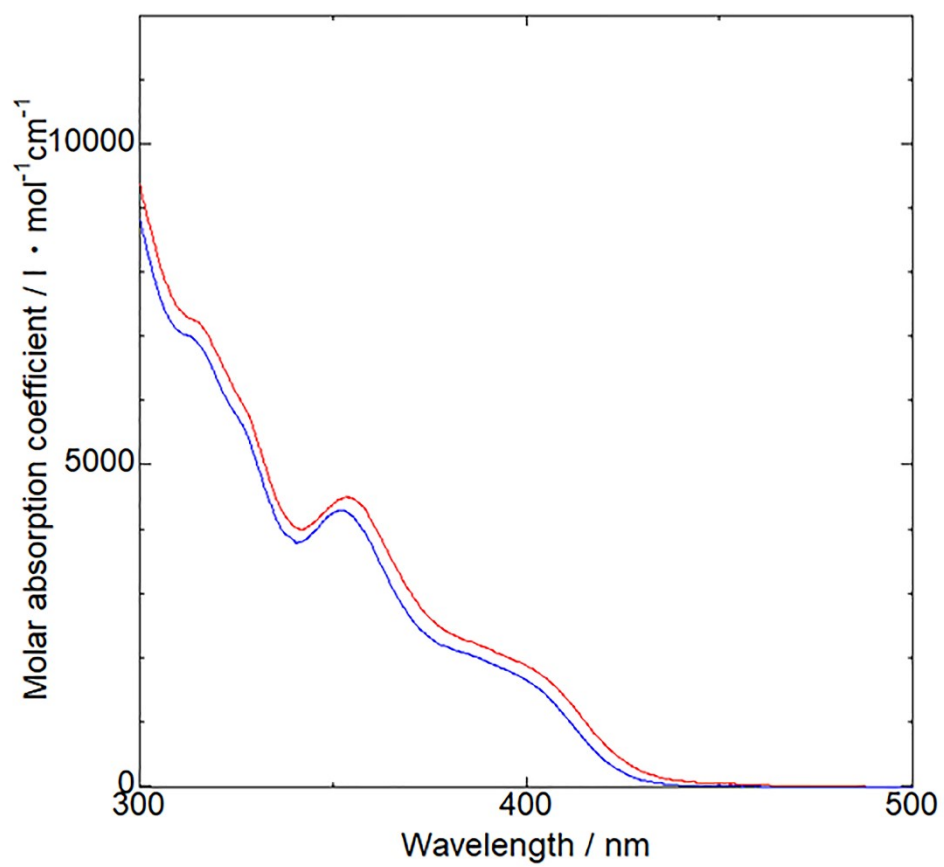


Figure S9. Absorption spectra of **1** in DMA (red, 1.85×10^{-5} M) and DMF (blue, 2.46×10^{-5} M) solution.

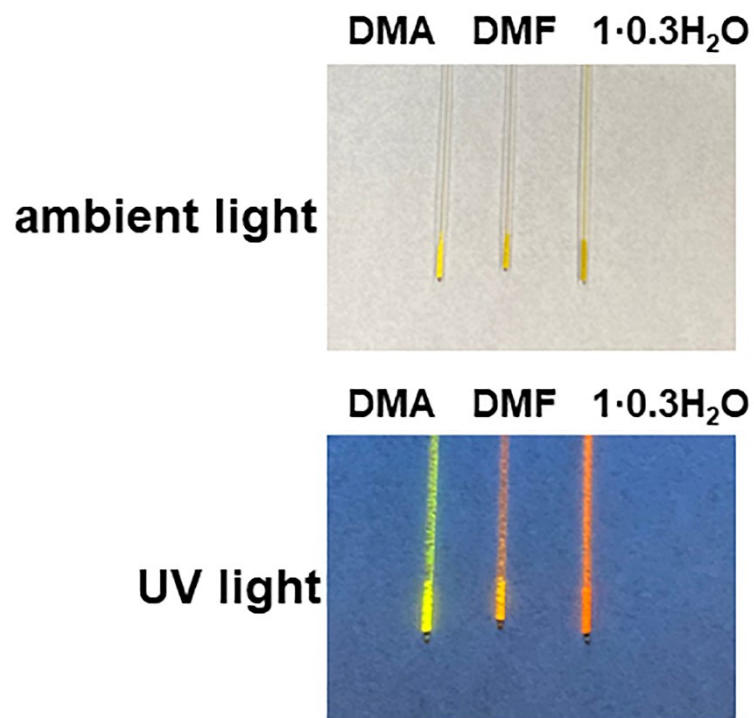


Figure S10. Photographs of $1 \cdot 0.3\text{H}_2\text{O}$ compared with DMF and DMA vapor exposure under ambient light (top) and UV light irradiation (bottom).

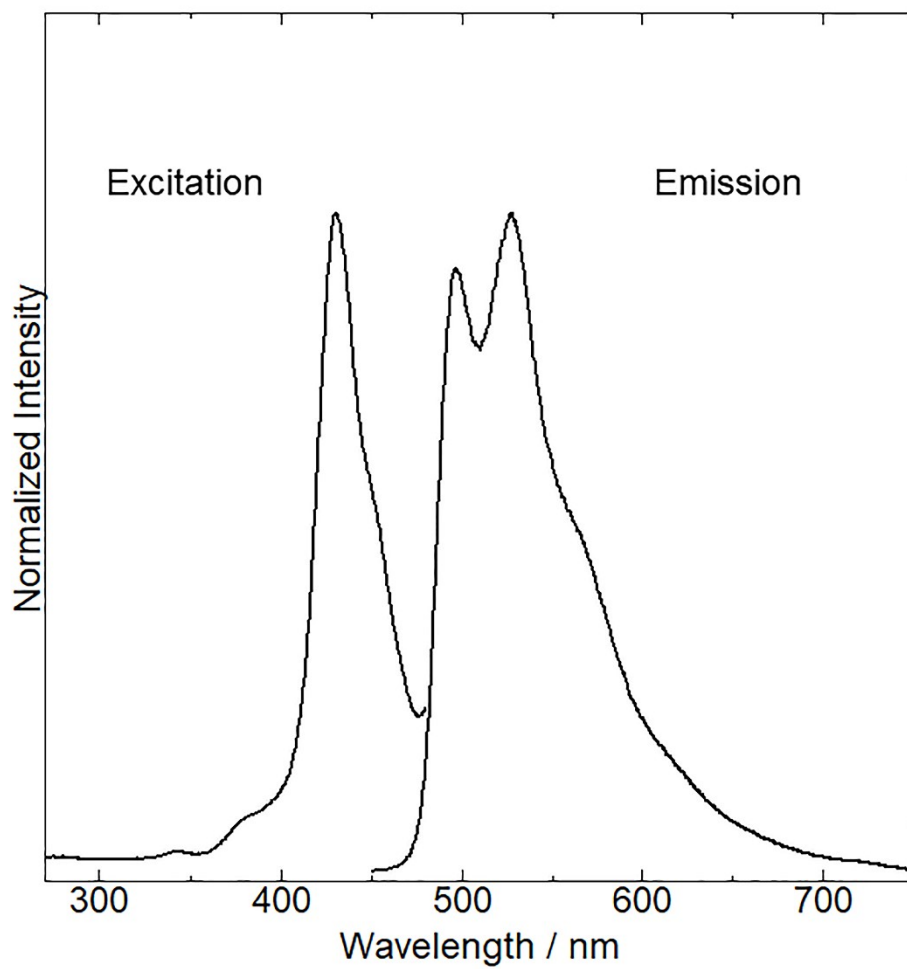


Figure S11. Emission ($\lambda_{\text{ex}}=400$ nm) and excitation ($\lambda_{\text{em}}=527$ nm) spectrum of **1** in DMA solution.

Table S1. Selected bond length and intermolecular Pt···Pt interactions of **1·3DMA** and **1·0.75DMF** at 90 K.

Complex	1·3DMA	1·0.75DMF
Pt1-N1	2.070(3) Å	2.08(1) Å
Pt1-C1	2.027(3) Å	2.01(1) Å
Pt1-C12	1.942(4) Å	1.97(1) Å
Pt1-C13	2.027(3) Å	2.01(2) Å
Pt2-N4	-	2.04(1) Å
Pt2-C14	-	2.05(1) Å
Pt2-C25	-	1.93(2) Å
Pt2-C26	-	2.03(1) Å
Pt1···Pt1	7.4967(3) Å	-
Pt1···Pt2	-	3.4765(6) Å, 6.7976(7) Å
Pt3-N7	-	2.05(1) Å
Pt3-C27	-	2.04(1) Å
Pt3-C38	-	1.96(1) Å
Pt3-C39	-	2.01(1) Å
Pt4-N10	-	2.05(1) Å
Pt4-C40	-	2.03(1) Å
Pt4-C51	-	1.95(2) Å
Pt4-C52	-	2.03(1) Å
Pt3···Pt4	-	3.3714(7) Å, 6.9444(7) Å

Table S2. Comparison for possible molecular composition and that found from elemental analysis.

composition	C (%)	H (%)	N (%)
1·0.1H ₂ O	30.55	1.22	8.22
1·0.2H ₂ O	30.44	1.26	8.19
1·0.3H ₂ O	30.34	1.29	8.16
1·0.4H ₂ O	30.23	1.33	8.14
1·0.5H ₂ O	30.13	1.36	8.11
1·0.6H ₂ O	30.02	1.40	8.08
1·0.7H ₂ O	29.92	1.43	8.05
1·0.8H ₂ O	29.81	1.46	8.02
1·0.9H ₂ O	29.71	1.50	8.00
Found from Elemental analysis	30.19	1.45	8.09

Table S3. Lattice constant refinement result for **1** after DMA and DMF vapor exposure compared with the single crystals.

\square	a / Å	b / Å	c / Å	$\alpha / ^\circ$	$\beta / ^\circ$	$\gamma / ^\circ$
1·3DMA single crystal	7.4967(2)	10.2891(3)	20.1177(5)	79.821(1)	87.171(1)	74.152(1)
DMA vapor exposure	7.580(7)	10.47(1)	20.18(2)	79.75(5)	87.65(5)	73.57(4)
1·0.75DMF single crystal	41.7895(9)	8.5044(2)	21.2104(4)	90	107.837(1)	90
DMF vapor exposure	41.969(9)	8.616(2)	21.503(3)	90	108.42(2)	90