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Supporting Information

Proton-Switchable Vapochromic Behaviour of a Platinum(II)-Carboxy-Terpyridine Complex

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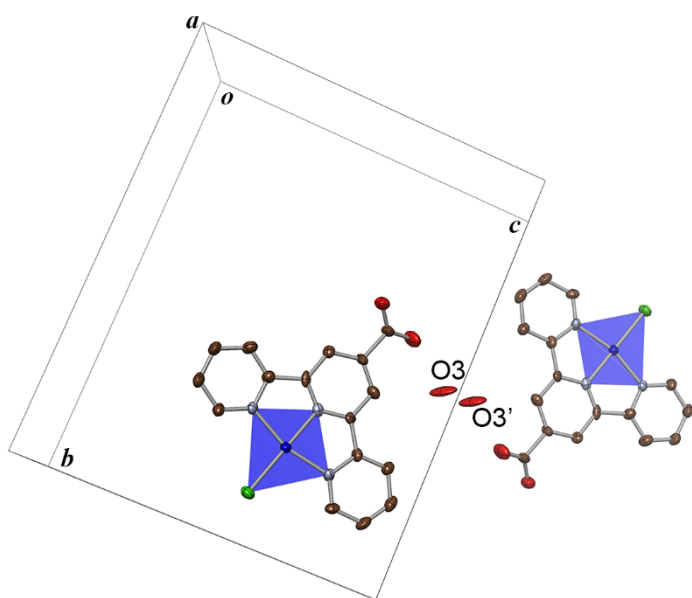


Figure S1. The positions of disordered water molecules between the adjacent two complex molecules in $1 \cdot 3.5\text{H}_2\text{O}$.

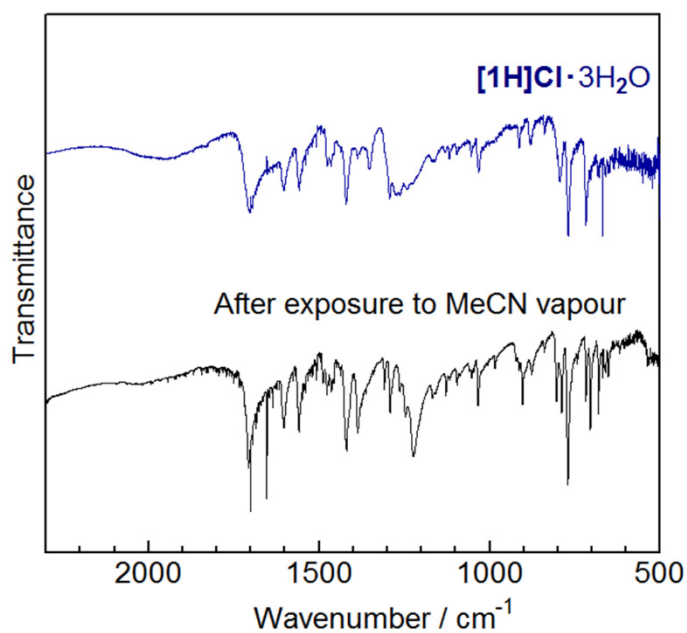


Figure S2. IR spectra of $[1\text{H}]\text{Cl} \cdot 3\text{H}_2\text{O}$ before and after exposure to MeCN vapour for 3 days at room temperature.

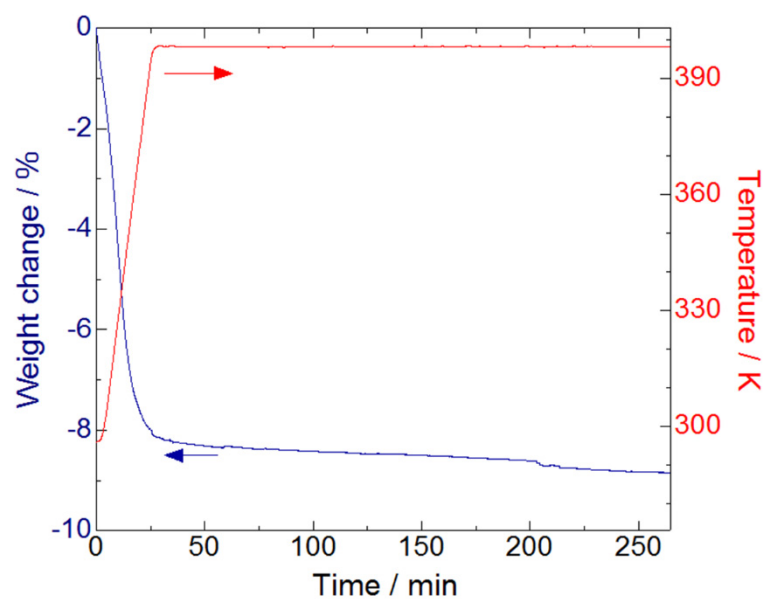


Figure S3. Thermogravimetric analysis for $[1\text{H}]\text{Cl}\cdot 3\text{H}_2\text{O}$ in N_2 atmosphere. Observed weight loss (8.8 % at 250 min heating) is quantitatively agreed with the amount of the three hydrated water molecules (9.0 %) in the $[1\text{H}]\text{Cl}\cdot 3\text{H}_2\text{O}$.

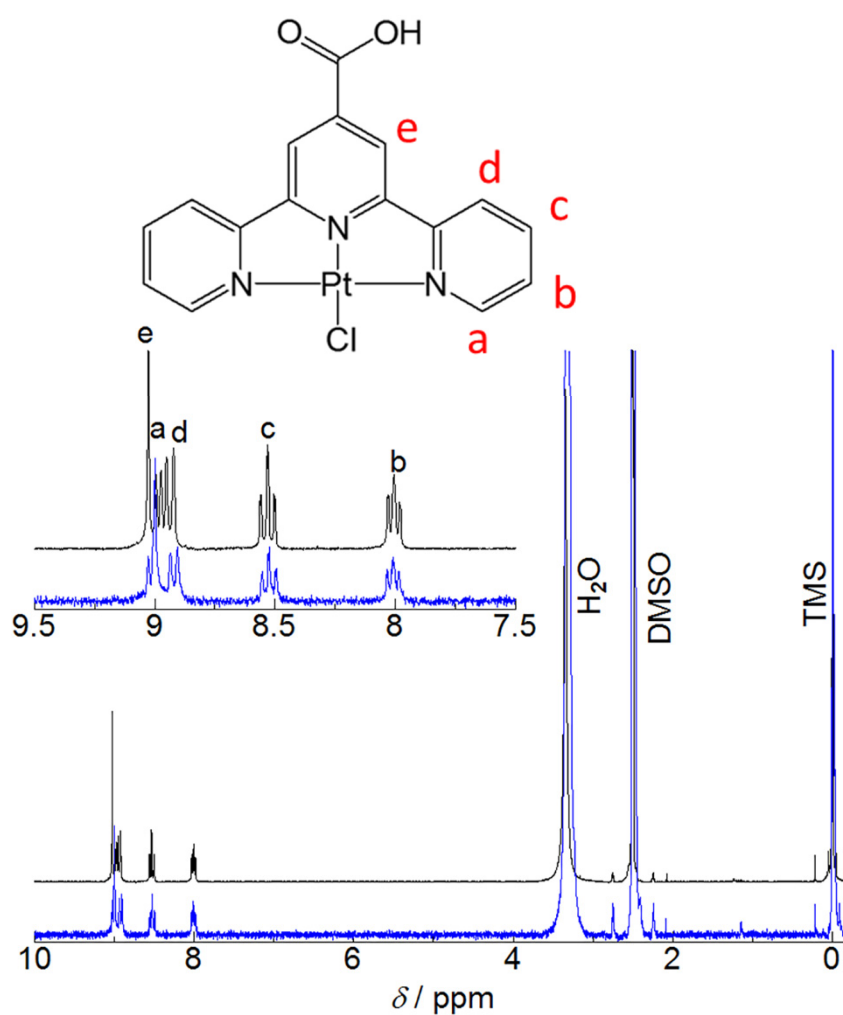


Figure S4. ^1H NMR spectra (DMSO- d_6) of as-synthesized **[1H]Cl**·3H₂O (blue) and after exposure to MeCN vapour for 3 days at room temperature (black). The inset shows the magnification of the aromatic region from 7.5 to 9.5 ppm. The signal of OH proton of carboxylic acid group was not observed probably due to the rapid exchange with protons of water molecules.

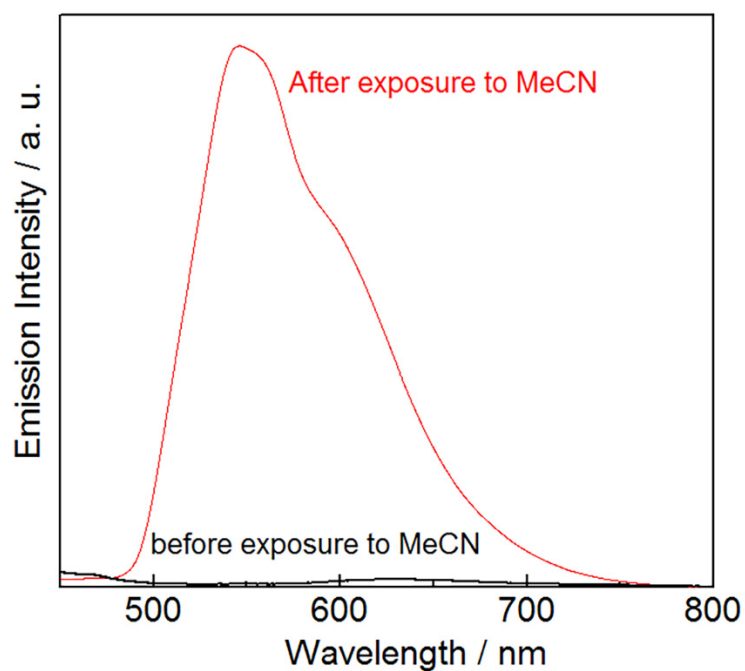


Figure S5. Change of luminescence spectrum of $[1\text{H}]\text{Cl}\cdot 3\text{H}_2\text{O}$ before (black) and after (red) exposure to MeCN vapour for 3 days at room temperature.

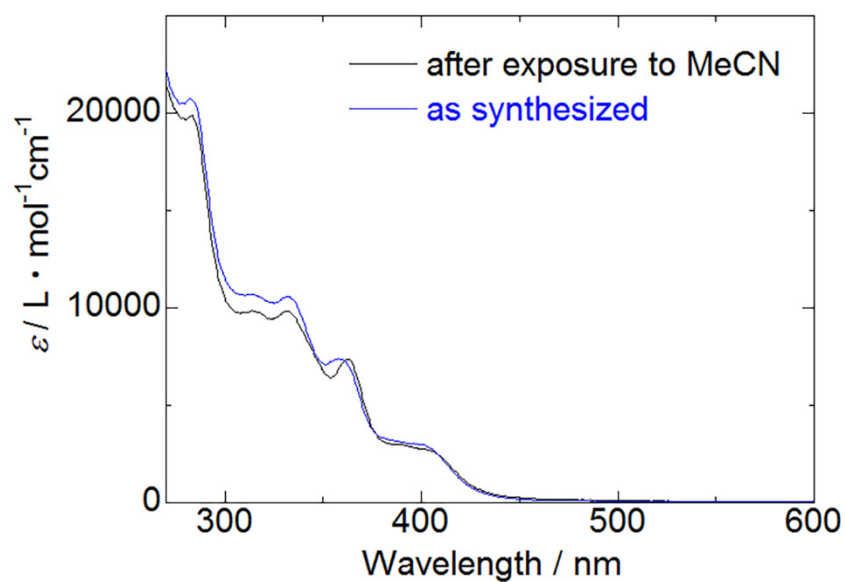


Figure S6. UV-Vis absorption spectra in DMSO of as-synthesized $[1\text{H}]\text{Cl}\cdot 3\text{H}_2\text{O}$ (blue) and after exposure to MeCN vapour for 3 days at room temperature (black).

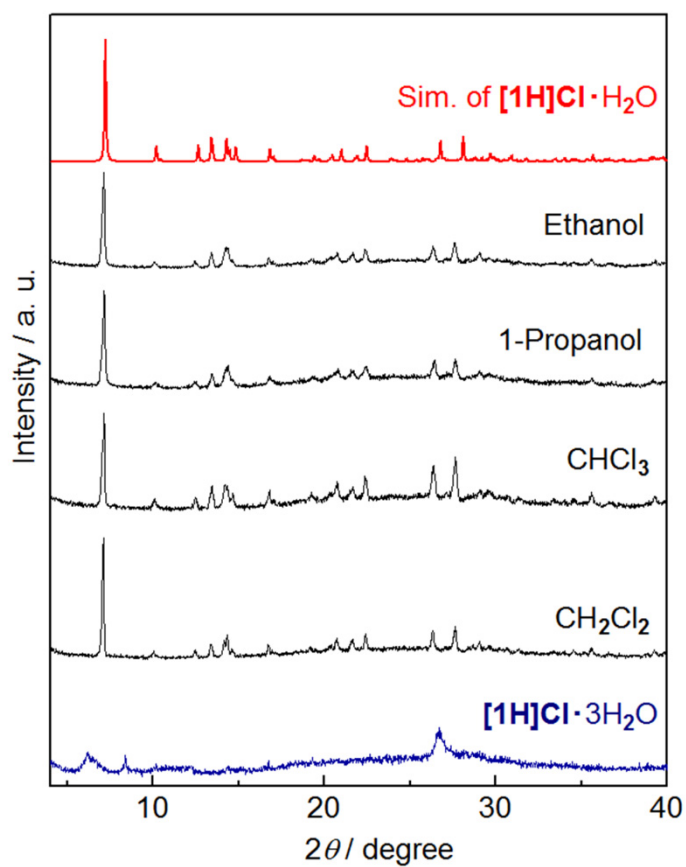


Figure S7. Changes of PXRD pattern of $[1H]Cl \cdot 3H_2O$ under exposing to various organic solvent vapours for 3 days at 30 °C. The top red line shows the simulation pattern calculated from the crystal structure of the protonated monohydrate $[1H]Cl \cdot H_2O$.

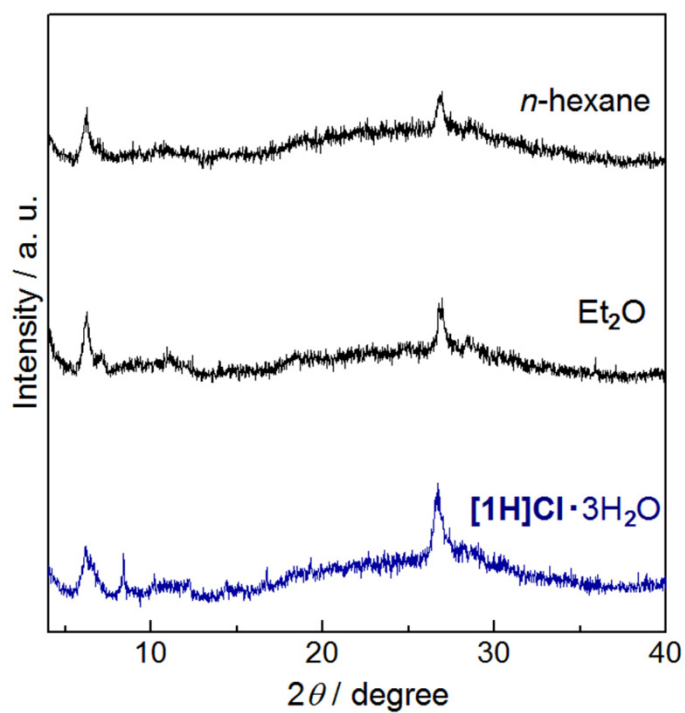


Figure S8. Changes of PXRD pattern of $[\text{1H}]\text{Cl} \cdot 3\text{H}_2\text{O}$ after exposure to Et_2O or hexane vapour for 3 days at 30 °C.

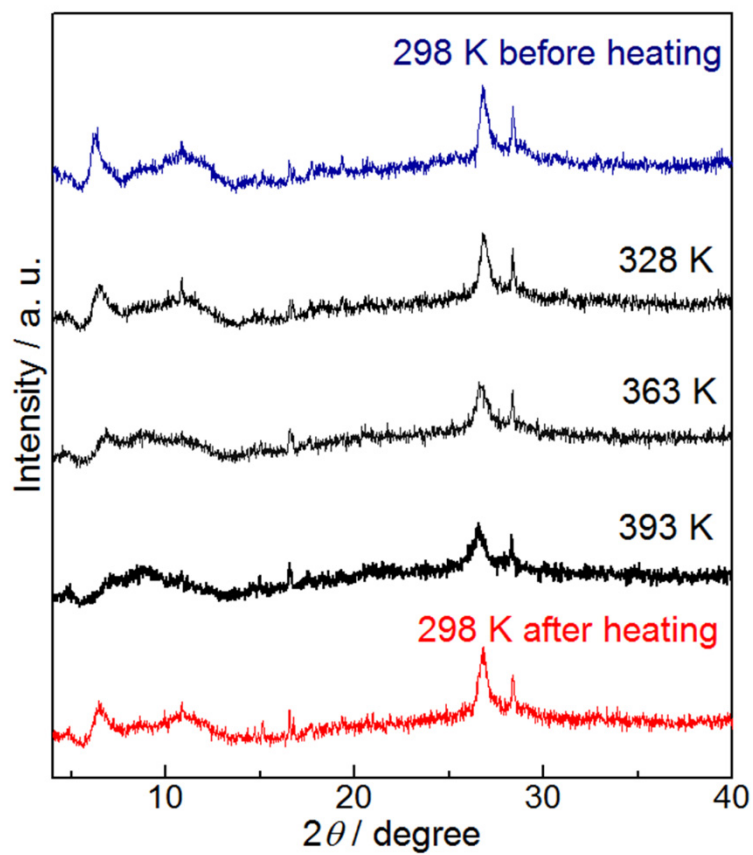


Figure S9. Temperature-dependence of PXRD pattern of $[1H]Cl \cdot 3H_2O$.

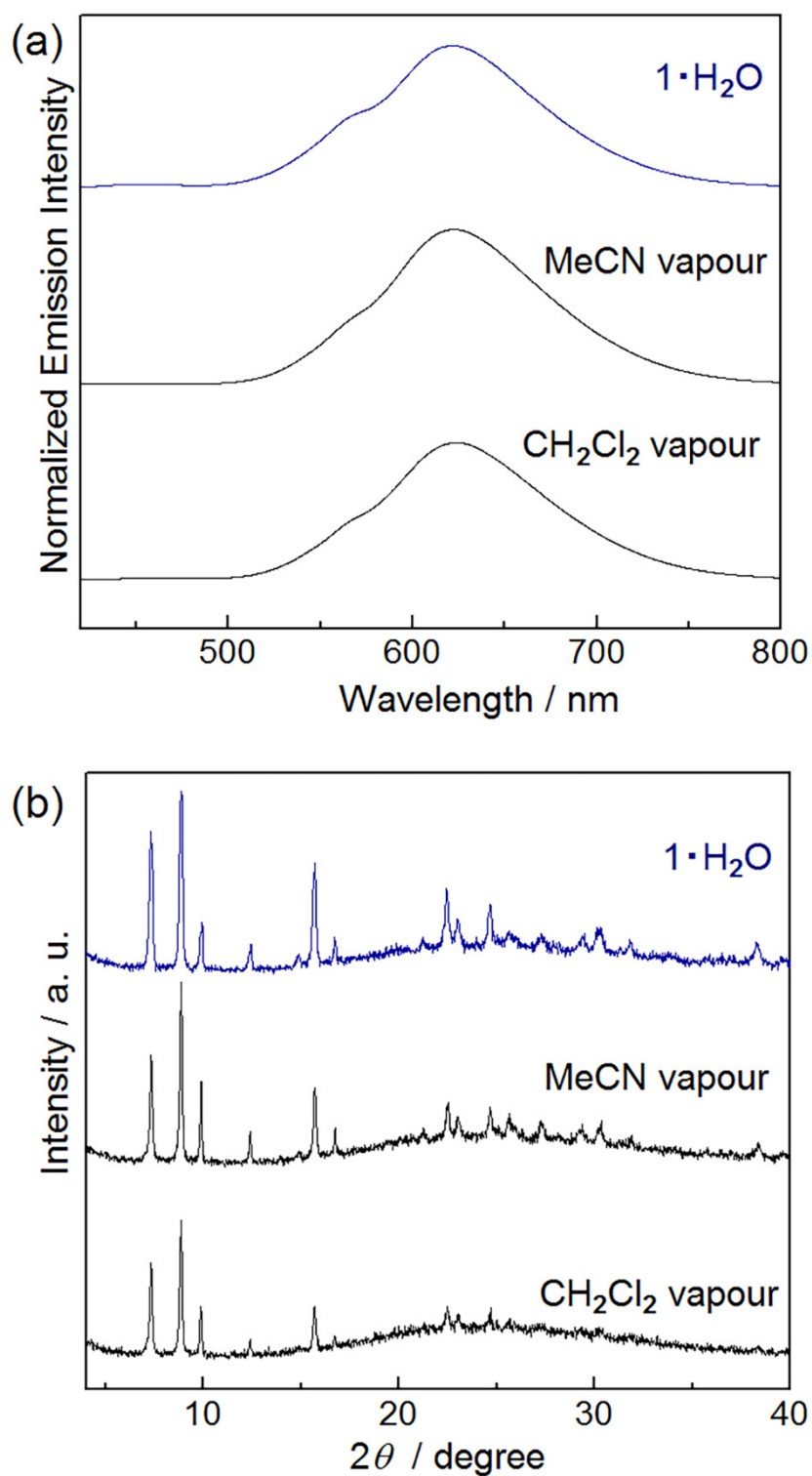


Figure S10. Changes of (a) luminescence spectrum and (b) PXRD pattern of $1 \cdot \text{H}_2\text{O}$ by exposing it to MeCN or CH_2Cl_2 vapour for 3 days at 30 °C.

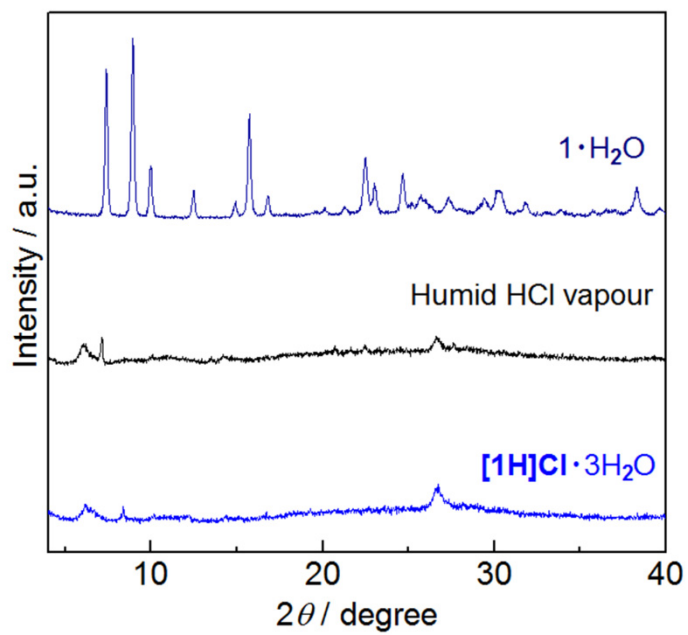


Figure S11. Changes of PXRD pattern of $1 \cdot \text{H}_2\text{O}$ by exposing it to humid HCl vapour for 3 days at 30 °C. The bottom blue line shows the PXRD pattern of $[\text{1H}]\text{Cl} \cdot 3\text{H}_2\text{O}$.

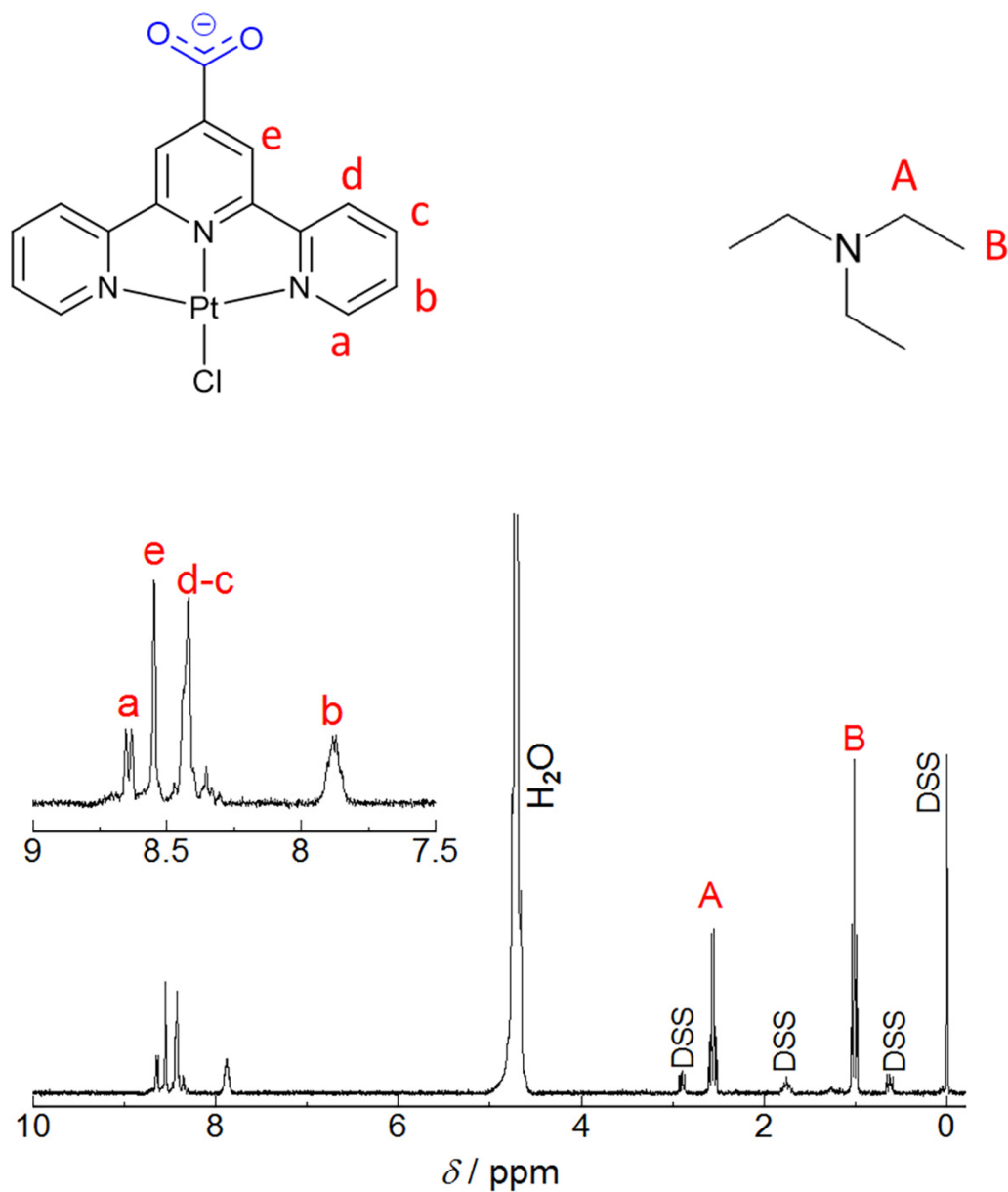


Figure S12. ^1H NMR spectrum of **[1H]Cl**·3H₂O after exposing it to triethylamine vapour (4%ND₃ in D₂O). The inset shows the magnification of the aromatic region from 7.5 to 9.0 ppm. The ratio of integral intensities of the signals B to b is 9 : 2, indicating the formation of the equimolar amount of the complex **1** and [TEA-H]⁺Cl⁻.

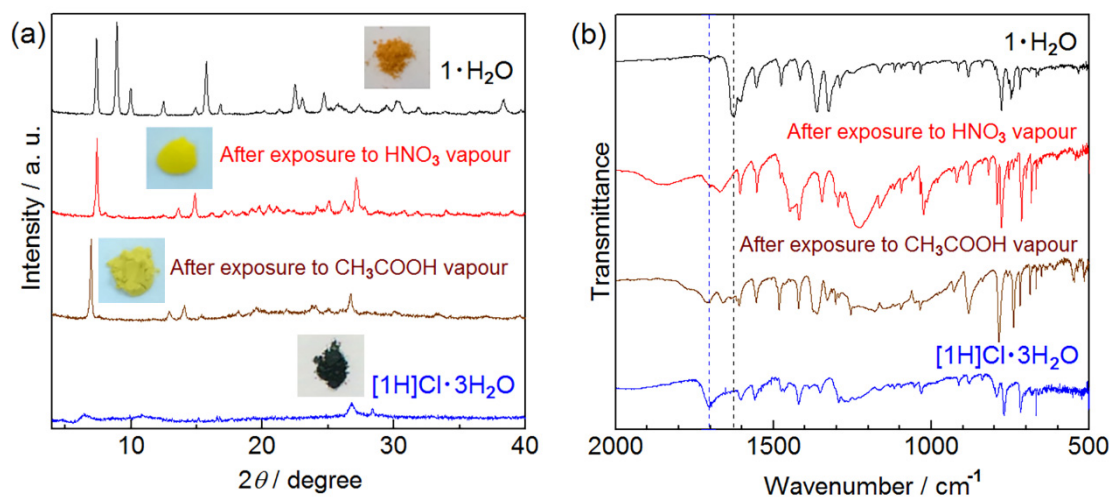


Figure S13. Changes of (a) PXRD pattern and (b) IR spectrum of $1 \cdot \text{H}_2\text{O}$ under exposure to humid HNO_3 or CH_3COOH vapour at room temperature. The bottom blues lines show the pattern and spectrum of the dark-blue protonated form $[\text{1H}]\text{Cl} \cdot 3\text{H}_2\text{O}$. The blue and black dotted lines in (b) indicate the positions of the $\nu(\text{C}=\text{O})$ modes of carboxy groups of protonated $[\text{1H}]\text{Cl} \cdot 3\text{H}_2\text{O}$ and deprotonated $1 \cdot \text{H}_2\text{O}$, respectively.