Supporting Information

H-bond-induced luminescence enhancement in Pt₁Ag₃₀ nanocluster and its application in methanol detection

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This Supporting Information includes: Figures S1-S20 Tables S1-S2



Figure S1. Schematic diagram of the crystallization process of Pt₁Ag₃₀.



Figure S2. The unit cell of $[Pt_1Ag_{30}(SAdm)_{14}(Bdpm)_4Cl_5](BPh_4)_3$ (Color labels: blue = Ag; dark green = Pt; red = S; purple = P; yellow = B; dark grey = N).

To confirm the optimal excitation wavelength, the excitation spectra for the emission bands at 640 nm and 710 nm were measured, respectively (Figure S3 a). As shown in Figure S3 a, there are two excitation wavelengths located at 525 nm and 440 nm. Then, the 440 nm and 525 nm were employed as excitation wavelengths to measure the emission intensity of Pt_1Ag_{30} dissolved in DCM, respectively. As shown in Figure S3 b, the intensity of photoluminescence is higher with the excitation wavelength at 440 nm than that at 525 nm. So, 440 nm was chosen as the optimal excitation wavelength for the photoluminescence test of the Pt_1Ag_{30} nanocluster in this study.



Figure S3. (a) The PL excitation spectra for the emission bands at 640 nm and 710 nm. (b) The PL emission spectra of Pt_1Ag_{30} dissolved in DCM with the excitation wavelength of 440nm and 525 nm, respectively.



Figure S4. Time-correlated single-photon counting trajectories of Pt₁Ag₃₀ in ACN.



Figure S5. Time-correlated single-photon counting trajectories of Pt₁Ag₃₀ DMF.



Figure S6. Time-correlated single-photon counting trajectories of Pt₁Ag₃₀ in acetone.



Figure S7. Time-correlated single-photon counting trajectories of Pt_1Ag_{30} in TCM.



Figure S8. Time-correlated single-photon counting trajectories of Pt₁Ag₃₀ in THF.



Figure S9. PL spectrum of Pt_1Ag_{30} in a solid state.



Figure S10. PL spectrum of Pt_1Ag_{30} in single crystal state.



Figure S11. DLS measurement result of Pt_1Ag_{30} dissolved in DCM, DMF, TCM, THF, EtOH, and ACN.



Figure S12. Fluorescence spectra tracing of adding H₂O to MeOH solution of Pt₁Ag₃₀.



Figure S13. Fluorescence spectra tracing of adding H_2O to ACN solution of Pt_1Ag_{30} .



Figure S14. Fluorescence spectra tracing of adding H_2O to DCM solution of Pt_1Ag_{30} .



Figure S15. Fluorescence spectra tracing of adding H_2O to TCM solution of Pt_1Ag_{30} .



Figure S16. Fluorescence spectra tracing of adding H_2O to THF solution of Pt_1Ag_{30} .



Figure S17. (a) Emissions and UV-Vis spectra of ACN solution of Pt_1Ag_{30} before adding H_2O , after adding H_2O , and after adding GH. (b) Photos of acetone solution under sunlight and UV-lamp in three states.



Figure S18. (a) Emissions and UV-Vis spectra of an acetone solution of Pt_1Ag_{30} before adding H_2O , after adding H_2O , and after adding GH. (b) Photos of acetone solution under sunlight and UV-lamp in three states.



Figure S19. (a) Emissions and UV-Vis spectra of DMF solution of Pt_1Ag_{30} before adding H_2O , after adding H_2O , and after adding GH. (b) Photos of DMF solution under sunlight and UV-lamp in three states.



Figure S20. Structure diagram of Bdpm (a) and DPPM (b).

Table S1. Fluorescence quantum yield of Pt_1Ag_{30} in different solvents.

| Solvent | QY |
|---------|--------|
| MeOH | 15.36% |
| EtOH | 2.18% |
| MeCN | 3.08% |
| DCM | 0.79% |
| ТСМ | 0.31% |
| Acetone | 0.26% |
| DMF | 0.21% |
| THF | 0.13% |

| CCDC | 2208493 |
|--|--|
| Empirical formula | $C_{333}H_{398}Ag_{30}B_3CI_{33}N_4P_8PtS_{14}\\$ |
| Formula weight | 9786.97 |
| Temperature/K | 150 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 21.6934(3) |
| b/Å | 23.8539(3) |
| c/Å | 34.4020(5) |
| α/° | 96.7550(10) |
| β/° | 100.9060(10) |
| γ/° | 100.2480(10) |
| Volume/Å ³ | 16989.5(4) |
| Z | 2 |
| ρ _{calc} g/cm ³ | 1.913 |
| µ/mm⁻¹ | 18.211 |
| F(000) | 8908.0 |
| Crystal size/mm ³ | 0.35 × 0.3 × 0.1 |
| Radiation | CuKα (λ = 1.54186) |
| 20 range for data collection/ 9.46 to 133.206 | |
| Index ranges | $-16 \le h \le 25, -25 \le k \le 28, -40 \le l \le 40$ |
| Reflections collected | 124446 |
| Independent reflections | 56983 [R _{int} = 0.0403, R _{sigma} = 0.0469] |
| Data/restraints/parameters | 56983/1965/3521 |
| Goodness-of-fit on F ² | 1.025 |
| Final R indexes [I>=2σ (I)] | R ₁ = 0.0613, wR ₂ = 0.1672 |
| Final R indexes [all data] | $R_1 = 0.0777, wR_2 = 0.1779$ |
| Largest diff. peak/hole / e Å ⁻³ 3.20/-1.42 | |

Table S2 Crystal data and structure refinement for Pt₁Ag₃₀.