A multifunction photochromic metal-organic framework with Lewis acid sites for selective amines and anion sensing

Jian-Jun Liu,^a* Qi-Tao Que,^a Dan Liu,^a Hongbo Suo^b, Jiaming Liu^c and Shu-Biao Xia *^a

 ^a Center for Yunnan-Guizhou Plateau Chemical Functional Materials and Pollution Control, Qujing Normal University, Qujing 655011, China
 ^b School of Pharmacy, Liaocheng University, Liaocheng, Shandong 252059, China
 ^c School of Metallurgy Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, PR China

E-mail: jjliu302@163.com; xiashubiao401@163.com

| Complex | 1 |
|---|--|
| Chemical formula | C ₃₆ H ₃₀ ClEuN ₄ O ₁₂ |
| formula weight | 898.05 |
| crystal system | Triclinic |
| space group | <i>P</i> -1 |
| <i>a</i> (Å) | 9.6088(7) |
| <i>b</i> (Å) | 14.6537(11) |
| <i>c</i> (Å) | 16.9619(14) |
| α (deg) | 95.8520(10) |
| β (deg) | 106.5110(10) |
| γ (deg) | 107.9380(10) |
| $V(Å^3)$ | 2131.0(3) |
| Ζ | 2 |
| $\rho_{calc}(g/cm^3)$ | 1.400 |
| μ (Mo Ka) (mm ⁻¹) | 1.594 |
| F(000) | 900 |
| collected reflns | 12867 |
| unique reflns/ R_{int} | 9270/ 0.0498 |
| no. of observations | 8142 |
| GOF | 1.047 |
| R_1^a , wR_2^b ($I > 2\sigma(I)$) | 0.0393, 0.1088 |
| $R_1^a, w R_2^b$ (all data) | 0.0456, 0.1129 |

Table S1. Crystallographic data and structure refinement details for 1.

^a $R_1 = \Sigma ||F_0| - |F_c|| / \Sigma |F_0|$. ^b $wR_2 = [\Sigma w (F_0^2 - F_c^2)^2 / \Sigma w (F_0^2)]^{1/2}$.



Fig. S1. TGA curve of complex 1.



Fig. S2. PXRD patterns of complex **1** after irradiation and soaking in $Cr_2O_7^{2-}$ anion solution.



Fig. S3. PXRD patterns of complex 1 after soaking in various amines.



Fig. S4. ESR spectrum of 1@dimethylamine in solid state.



Fig. S5. Emission spectra of complex 1 in solid state at room temperature.



Fig. S6. Emission spectra of complex 1 dispersed in various pure solvents (λ_{ex} = 390 nm).



Fig. S7. Families of various emission spectra of complex 1 in aqueous solution upon the addition of 0.2 mM of different selected anions (λ_{ex} = 390 nm).



Fig. S8. Comparison of the luminescence intensity of $Cr_2O_7^{2-}$ in the presence of mixed anions for complex 1.



Fig. S9. The UV-vis absorption spectrum of $Cr_2O_7^{2-}$ and the emission spectrum of complex 1.



Fig. S10. The UV-vis absorption spectra of anions and the excitation spectrum of complex 1.



Fig. S11. Photographs show the luminescence change of complex 1 in presence of $Cr_2O_7^{2-}$ (0.3 mM).



Fig. S12. XPS core level spectra of O and N atoms in complex 1.



Fig. S13. XPS for complex 1.