Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Lanthanide cation encapsulated in a metal-organic framework as a white LED and selective naked-eye reversible HCl sensor

*Huijun Li, Qingqing Li, Zhouqing Xu**

*College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo, Henan 454000, China, *Email - zhqxu@hpu.edu.cn.*

Table S1 Crystal data and structure refinement details of **HPU-14**[a].

Complex	**HPU-14**
Formula	$C_{39}H_{50}N_2O_{26}Zn_3$
formula weight, fw	1158.92
Temperature, *T* [K]	296(2)
crystal system	*Orthorhombic*
space group	*Pbca*
a [Å]	16.274(5)
b [Å]	10.787(3)
c [Å]	24.384(8)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	4281(2)
Z	4
ρ [g cm^{-3}]	1.798
μ [mm^{-1}]	1.770
θ range	1.67-28.48
F(000)	2384
goodness-of-fit, GOF	1.002
R_1[a] [I > 2σ (I)]	0.0432
wR_2[b] (all data)	0.0831

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

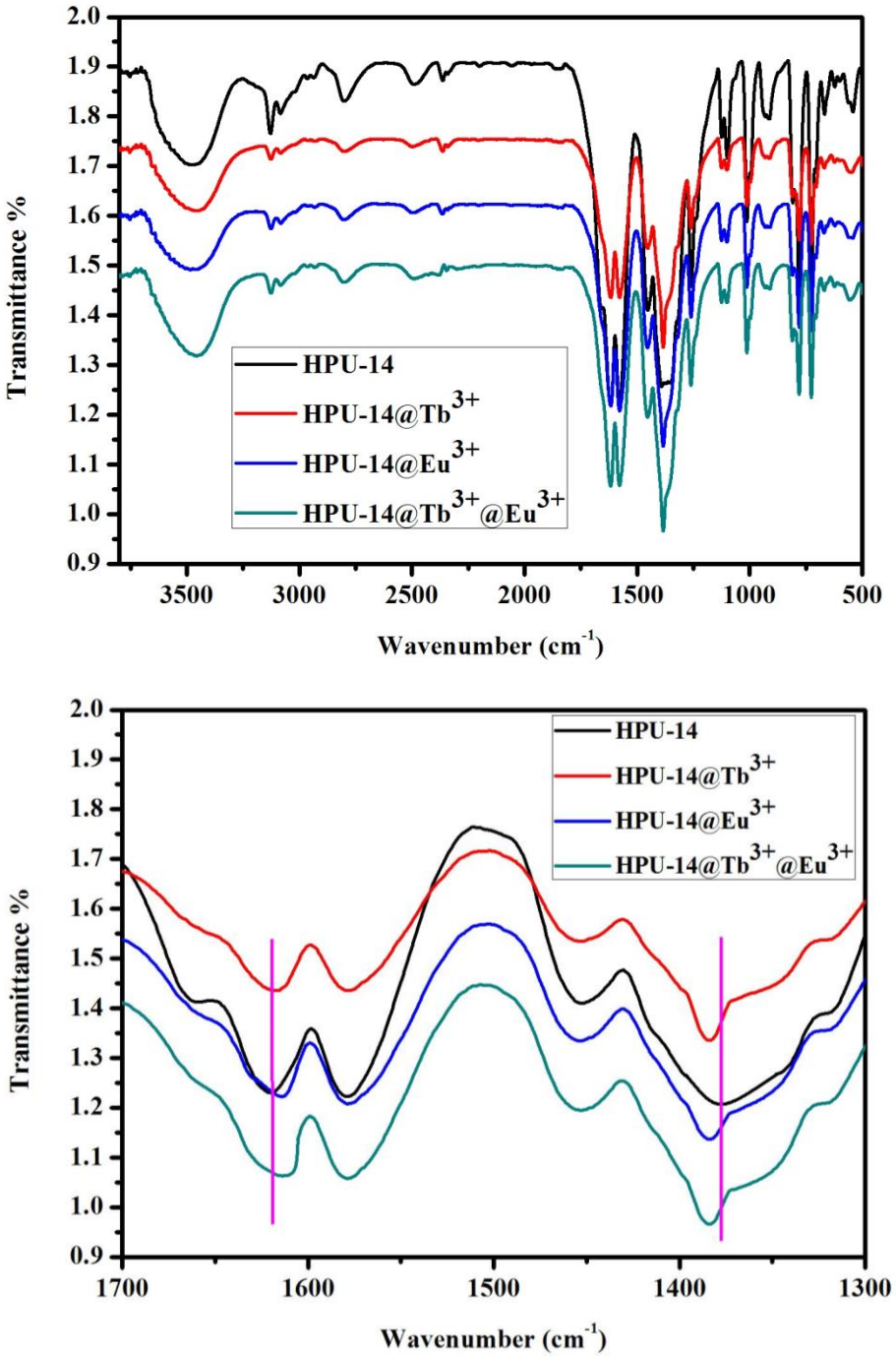

Figure S1 The IR spectra of **HPU-14**, HPU-14@Tb^{3+}, HPU-14@Eu^{3+}, and HPU-14@Tb^{3+}@Eu^{3+}.

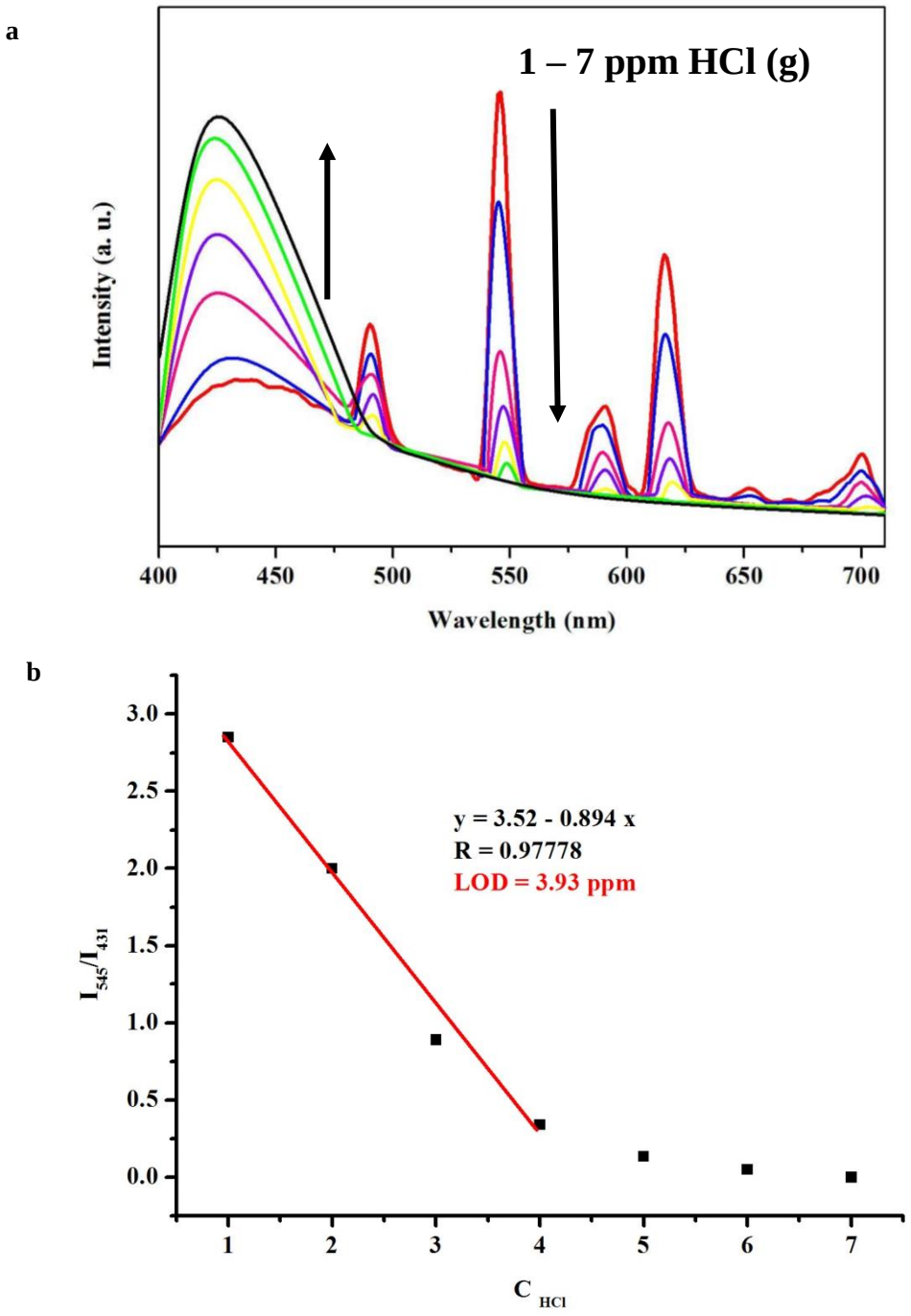

Figure S2 a: The emission spectra of HPU-14@Tb^{3+}@Eu^{3+} exposed to HCl gas with different concentrations; b: The plots of $I_{545}/_{431}$ *vs*. C_{HCl} with fitted curves in the range of 1-4 ppm.

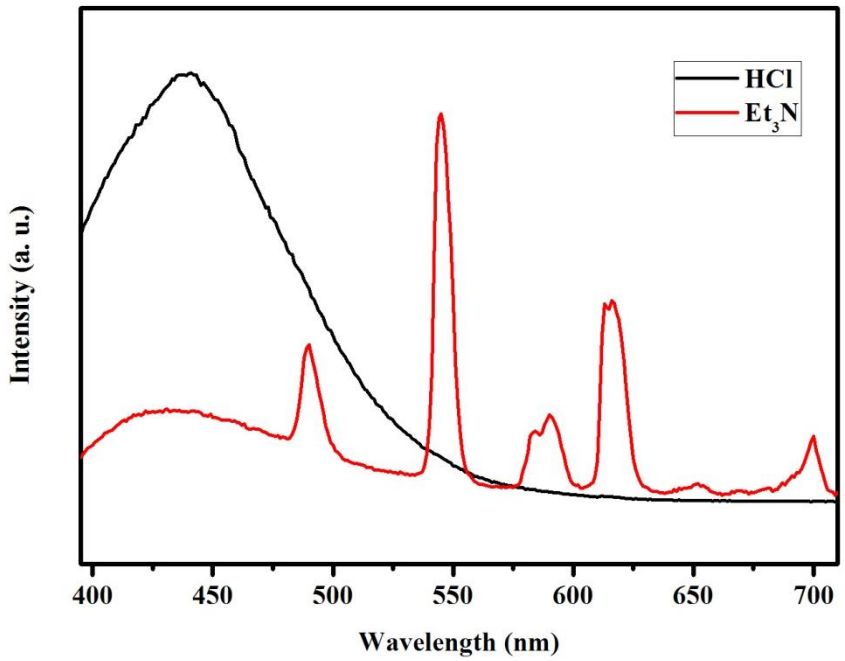

Figure S3 The emission spectra of HPU-14@Tb^{3+}@Eu^{3+} in HCl (g) and HCl-treated HPU-14@Tb^{3+}@Eu^{3+} in Et_3N (g).

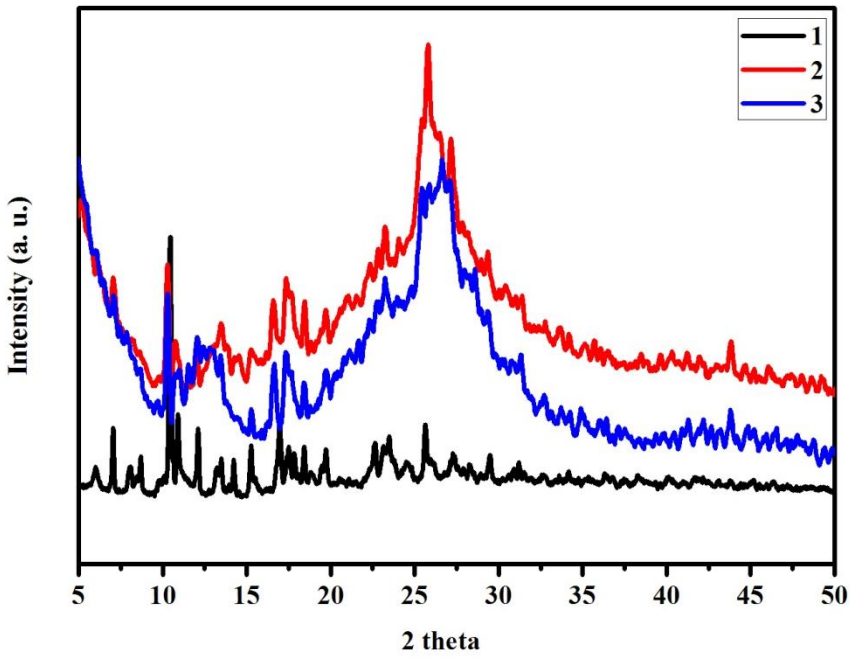

Figure S4 PXRD patterns of HPU-14@Tb^{3+}@Eu^{3+} (1), HPU-14@Tb^{3+}@Eu^{3+} in HCl (2) and HCl-treated HPU-14@Tb^{3+}@Eu^{3+} in Et_3N (3).

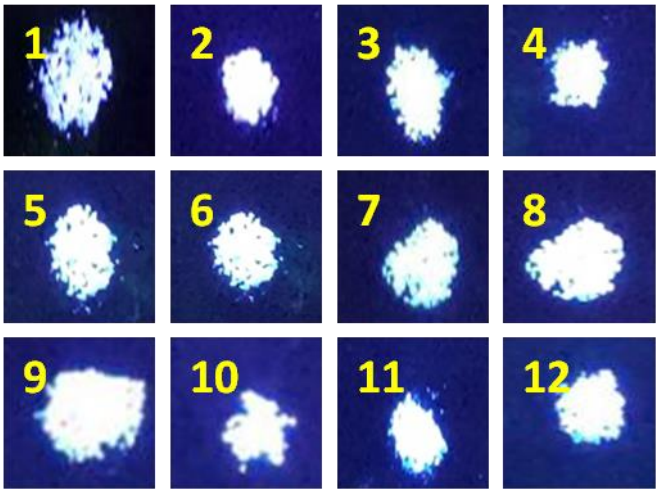

Figure S5 The luminescence image of **HPU-14@Tb^{3+}@Eu^{3+}** toward other common volatile toxic gaseous analogues. 1 HPU-14@Tb^{3+}@Eu^{3+}, 2 DMF, 3 DMA, 4 ethyl acetate, 5 trichloromethane, 6 acetonitrile, 7 ethanol, 8 methanol, 9 acetone, 10 styrene, 11 methylbenzene, 12 n-hexane.

Table S2 Luminescence lifetimes (μs) and quantum yields of HPU-14@Tb^{3+}@Eu^{3+}[a]

	τ_1 (μs)	τ_2 (μs)	τ_3 (μs)	τ_4 (μs)	<τ>(ms)	Φ
HPU-14@Tb@Eu	**5.27(1.87%)**	**46.84(2.98%)**	**308.33(26.27%)**	**797.55(68.87%)**	**0.733**	**7.1**

[a] $\langle\tau\rangle = \Sigma A_i\tau_1^2 / A_i\tau_1$

Table S3 The lifetime and quantum yield of other similar MOF-based materials.

	Quantum yield (%)	Lifetime (μs)
[Zn(μ-L)(μ-1,3-dpp)][1]	2.8	876
Mg-CP⊃CuI[2]	5.6	-
SMOF-1[3]	4.3	600
ZJU-1:1.5%Tb^{3+}, 2.0%Eu^{3+}[4]	6.8	
10% Eu-SMOF-1[5]	4.3	-

1 W. Huang, F. F. Pan, Y. Liu, S. D. Huang, Y. J. Li, J. Yong, Y. Li, A. M. Kirillov, and D. Y. Wu, Inorg. Chem. 2017, 56, 6362-6370

2 Z. F. Wu, B. Tan, Z. L. Xie, J. J. Fu, X. Y. Huang, J. Mater. Chem. C. 2016, 4, 2438.

3 D. F. Sava, L. E. S. Rohwer, M. A. Rodriguez, T. M. Nenoff, J. Am. Chem. Soc. 2012, 134, 3983.

4 X. Rao, Q. Huang, X. Yang, Y. Cui, Y. Yang, C. Wu, B. Chen, G. Qian, J. Mater. Chem. 2012, 22, 3210.

5 Wang, Z.; Wang, Z.; Lin, B.; Hu, X.; Wei, Y.; Zhang, C.; An, B.; Wang, C.; Lin, W. ACS Appl. Mater. Interfaces. 2017, 9, 35253-35259.