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

A novel cucurbit[6]uril-based supramolecular coordination assembly as a multiresponsive luminescent sensor for Fe^{3+}, $Cr_2O_7^{2-}$ and isoquinoline antibiotics in aqueous medium

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Crystallographic data for **1** has been deposited with the Cambridge Crystallographic Data Centre with No. CCDC 1903202. Copies of the data can be obtained free of charge via the Internet at http://www.ccdc.cam.ac.uk/conts/retrieving.html or by post at CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K. (Fax: 44-1223336033, E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for **1**

Compound	[Zn $(ACA)_4$]□CB[6]□[$NH_2(CH_3)_2$]□8H_2O

Empirical formula	$C_{100}H_{104}N_{26}O_{28}Zn$
Formula weight	2183.46
Crystal system	Monoclinic
Space group	C2/c
a (Å)	17.621(3)
b (Å)	21.874(3)
c (Å)	25.800(4)
α (°)	90
β (°)	105.875(4)
γ (°)	90
V (Å^3)	9565(3)
Z	4
D_c/(g cm^{-3})	1.516
μ/(mm^{-1})	0.355
F(000)	4560
θ range (°)	2.482-28.391
R_{int}	0.0774
Parameters	685
T (K)	298
goodness of fit	1.082
Limiting indices	$-23 \le h \le 23$
	$-29 \le k \le 29$
	$-34 \le l \le 34$
R indices [I > 2σ(I)]	R_1=0.0795, wR_2=0.1923
R indices (all data)	R_1=0.0933, wR_2=0.2034

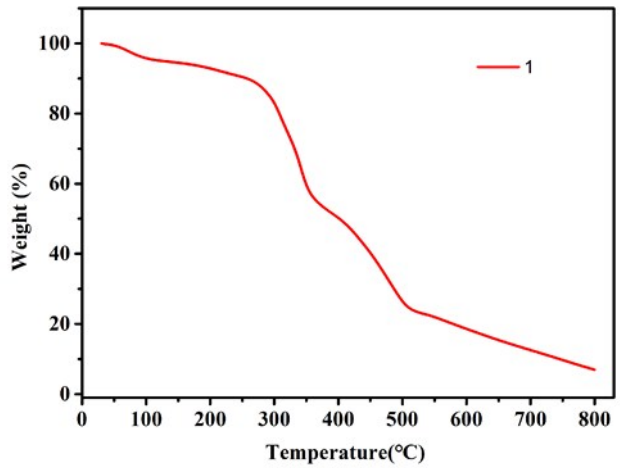

Fig. S1 TGA curves of 1 under an atmosphere of N_2 (5℃ min^{-1}).

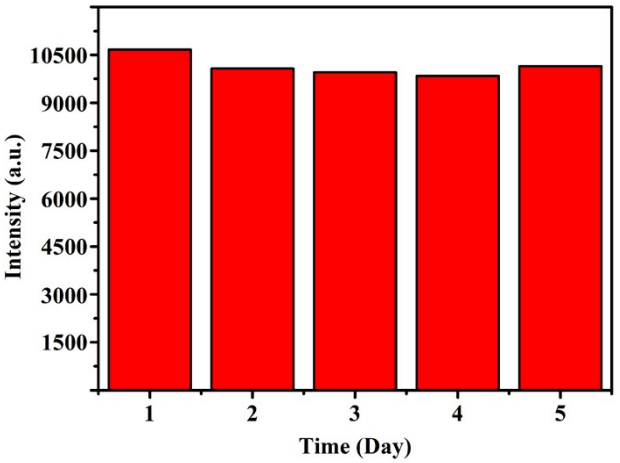

Fig. S2 Fluorescence spectra of 1 dispersed in water with different times.

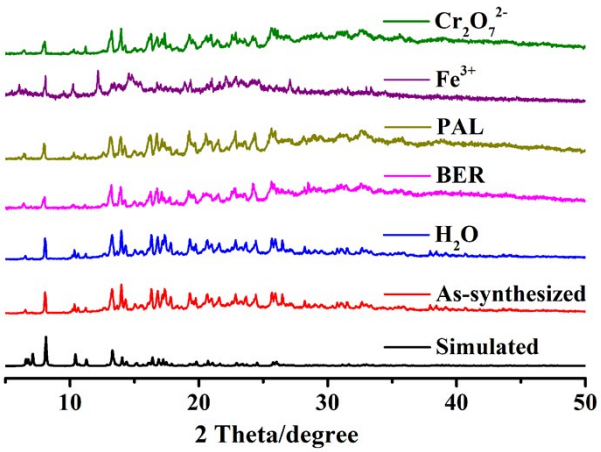

Fig. S3 PXRD patterns of **1** simulate, as-synthesized, and after immersed in H_2O, Fe^{3+}, $Cr_2O_7^{2-}$, PAL and BER for comparison.

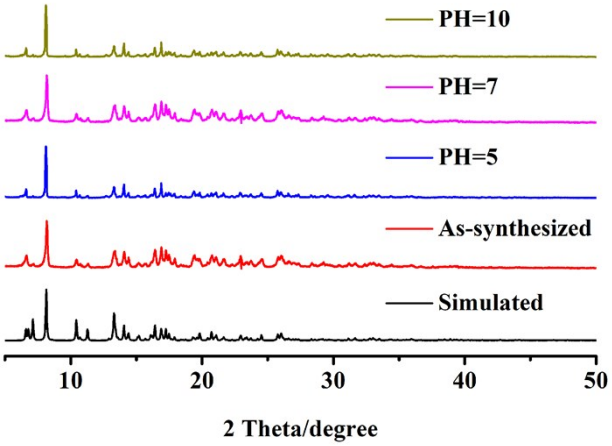

Fig. S4. PXRD patterns of **1** simulate, as-synthesized, and after treatment in acidic/alkaline aqueous solutions.

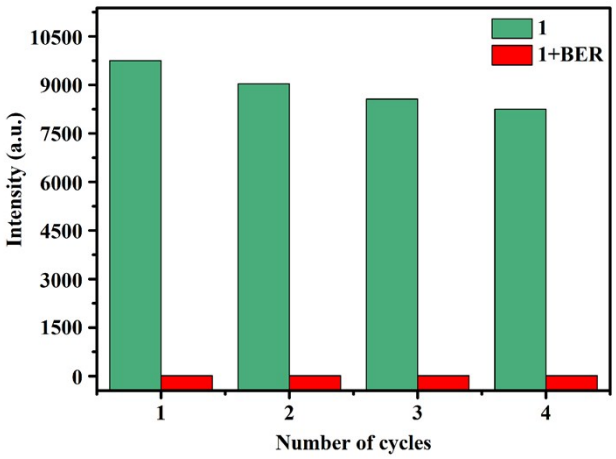

Fig. S5 Recyclability tests of **1** implemented with BER.

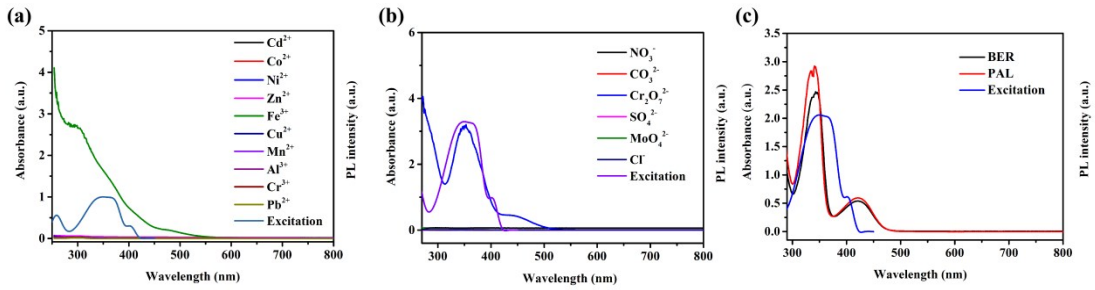

Fig. S6 UV-vis absorption spectra of different metal ions (a), inorganic anion (b),

antibiotics (c) in water, and excitation spectrum of **1**.

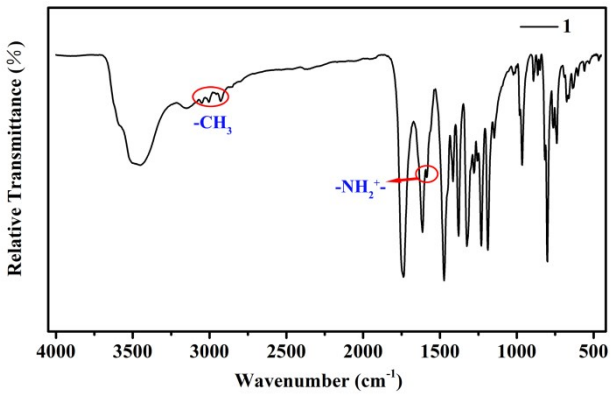

Fig. S7 IR spectra of **1**