Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Highly selective and sensitive colorimetric chemosensor for detection of Co^{2+} in a near-perfect aqueous solution

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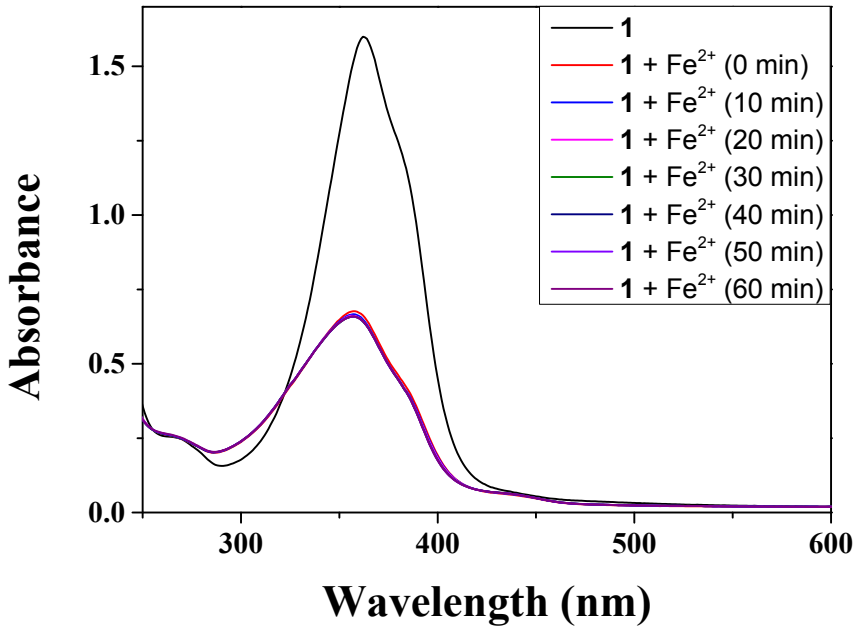


Fig. S1 Absorption spectral changes of **1** (20 μM) for 1 h in the presence of 1.1 equiv of Fe^{2+} ion in bis-tris buffer solution (10 mM, pH 7).

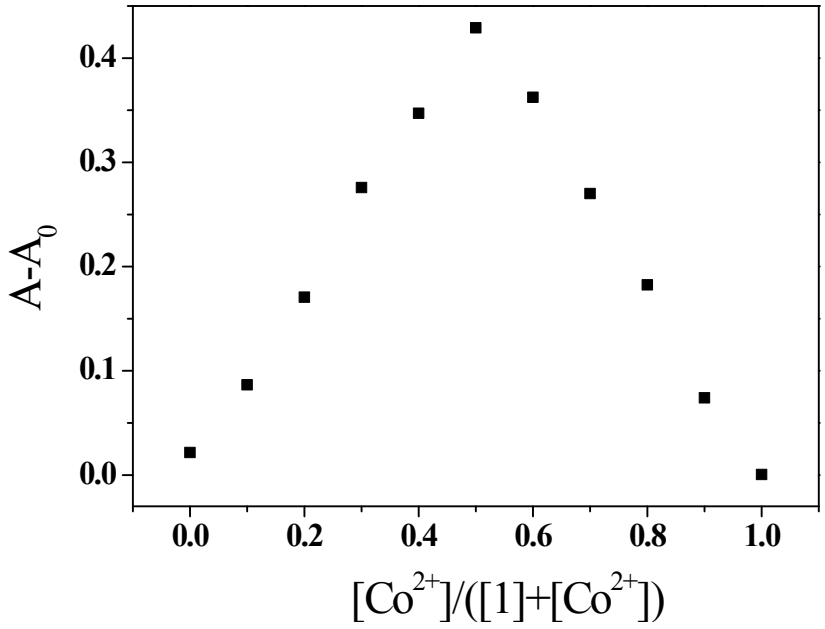


Fig. S2 Job plot of **1** and Co^{2+} in bis-tris buffer solution (10 mM, pH 7). The total concentrations of **1** and Co^{2+} were 150 μM.

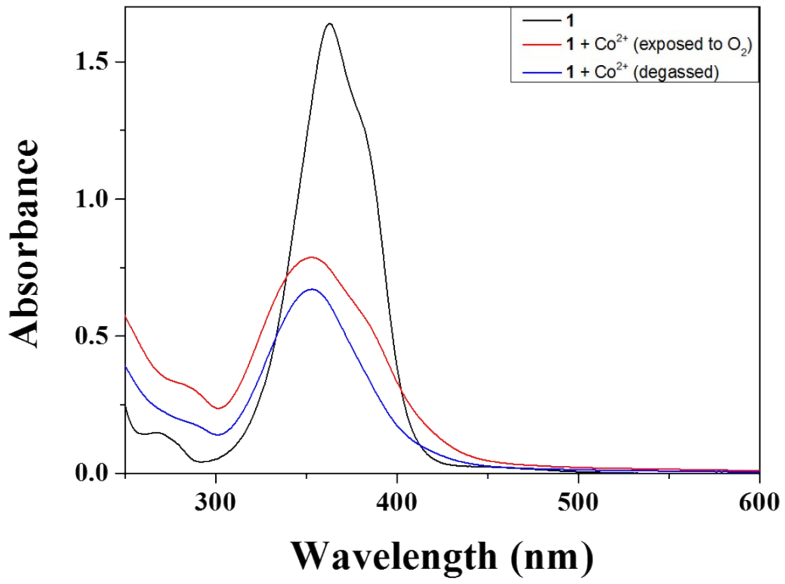


Fig. S3 Absorption spectra of **1** (20 μM) and **1**- Co^{2+} under the anaerobic and aerobic conditions, respectively.

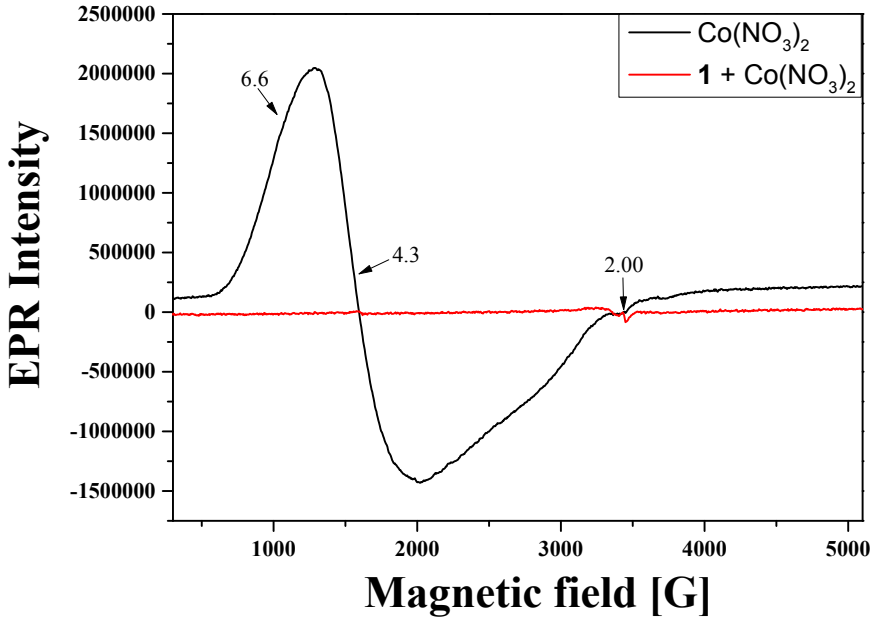


Fig. S4 X-band EPR spectra of $Co(NO_3)_2$ (black line) and **1** + $Co(NO_3)_2$ (red line) recorded at 5 K. Dark line: the $Co(NO_3)_2$ (1 mM) solution in CH_3CN (or H_2O) was frozen in liquid nitrogen. Red line: the EPR sample was frozen in liquid nitrogen 5 min after **1** (1.2 mM) was mixed with $Co(NO_3)_2$ (1 mM) in CH_3CN (or H_2O) at room temperature.

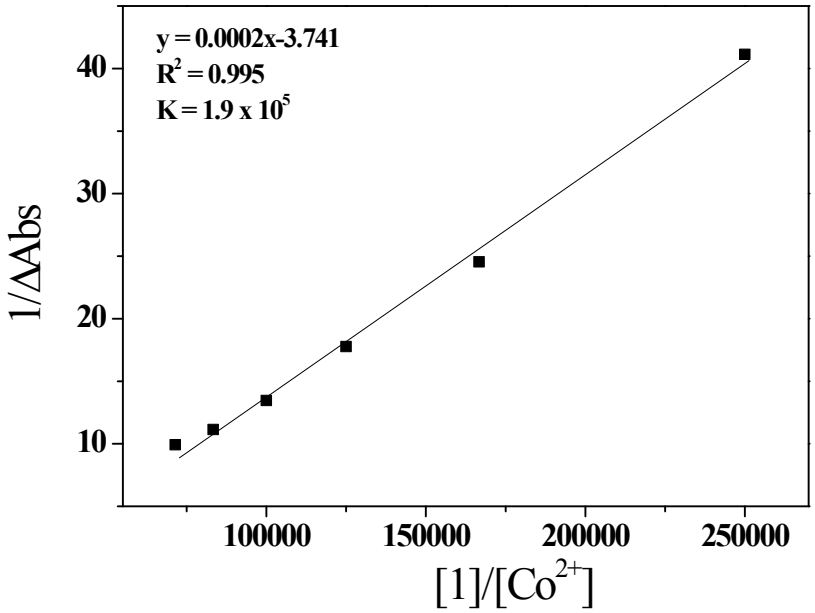


Fig. S5 Benesi-Hildebrand plot (absorbance at 420 nm) of **1** based on UV-vis titration, assuming 1:1 stoichiometry for association between **1** and Co^{2+}.

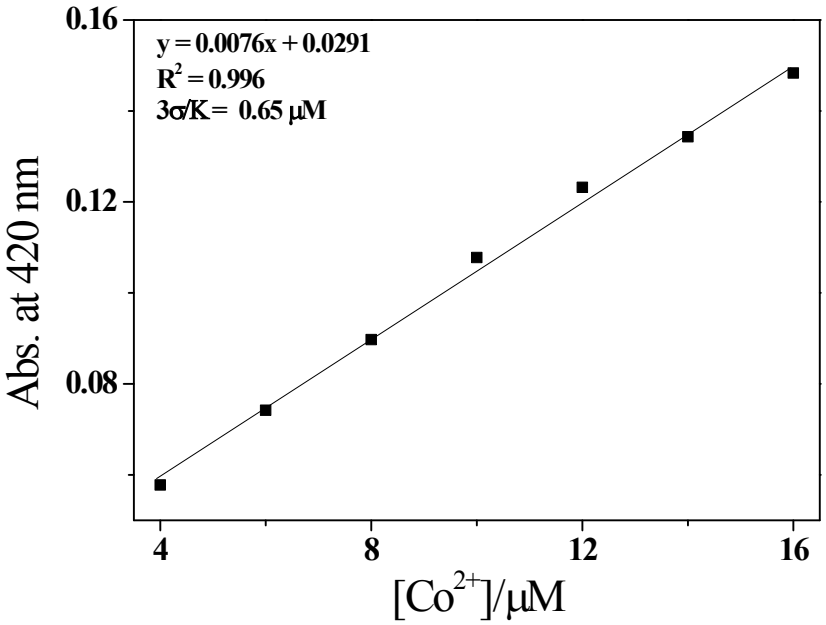
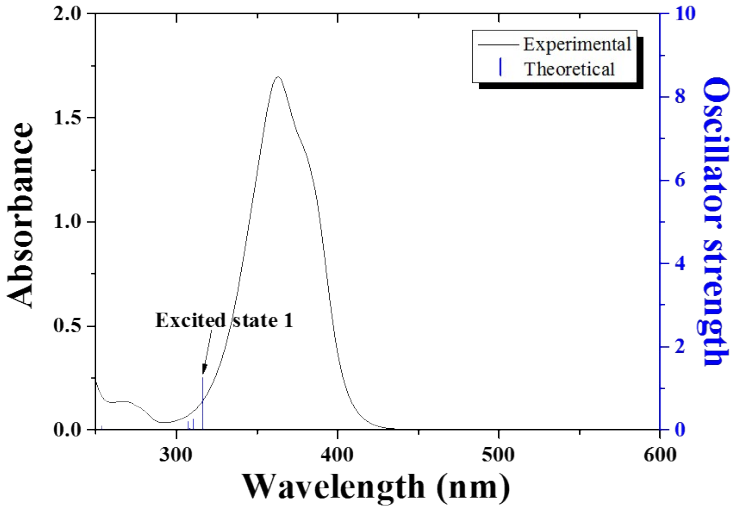


Fig. S6 Determination of the detection limit based on change in the ratio (absorbance at 420 nm) of **1** (20 μM) with Co^{2+}.

(a)

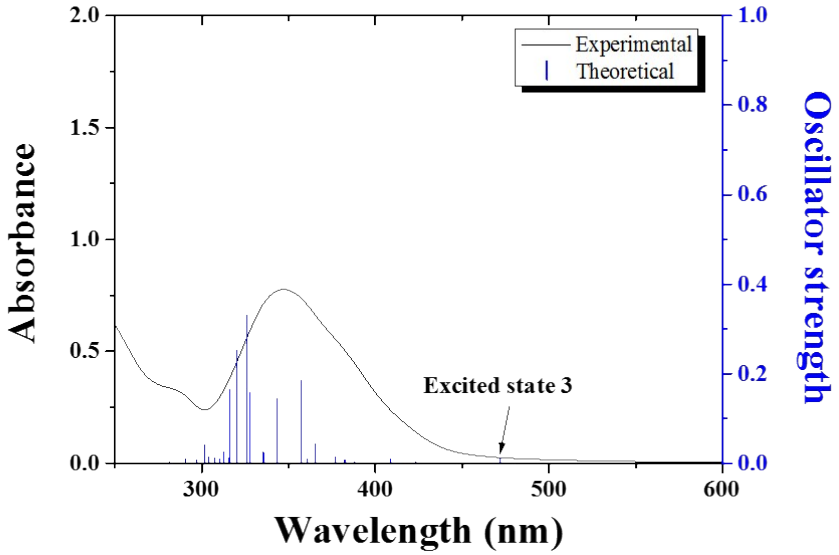


(b)

Excited state 1	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H → L	316.49	86	ICT	1.265
H - 1→ L + 1		12	ICT	

Fig S7. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energies and molecular orbital contributions for **1** (H = HOMO and L = LUMO).

(a)



(b)

Excited state 3	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H - 1 → L + 3	472.03	45	LMCT	0.0102
H - 8 → L + 3		15	LMCT	
H - 6 → L + 3		9	LMCT	
H - 14 → L + 3		3	LMCT	
H - 2 → L + 3		2	LMCT	

Fig. S8 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**-Co^{3+}. (b) The major electronic transition energies and molecular orbital contributions for **1**-Co^{3+} (H = HOMO and L = LUMO).