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Electronic Supplementary Information (ESI)

Zinc-based CPs for effectively detection of Fe^{3+} and $Cr_2O_7^{2-}$ ions

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Table S1 Selected Bond Distances (Å) and Angles (deg) for Complexes **1-4**.

		Complex **1**	
Zn1—O1	1.961 (3)	O1—Zn1—N2^{ii}	104.48 (15)
Zn1—O3^{i}	2.013 (4)	O3^{i}—Zn1—N2^{ii}	131.39 (17)
Zn1—N2^{ii}	2.046 (4)	O1—Zn1—N1	96.59 (15)
Zn1—N1	2.060 (4)	O3^{i}—Zn1—N1	113.31 (15)
Zn1—O4^{i}	2.457 (4)	N2^{ii}—Zn1—N1	103.91 (16)
O4—Zn1^{iii}	2.457 (4)	O1—Zn1—O4^{i}	158.33 (14)
O3—Zn1^{iii}	2.013 (4)	O3^{i}—Zn1—O4^{i}	57.24 (13)
N2—Zn1^{iv}	2.046 (4)	N2^{ii}—Zn1—O4^{i}	90.61 (15)
O1—Zn1—O3^{i}	101.20 (15)	N1—Zn1—O4^{i}	94.68 (15)
		Complex **2**	
Zn1—O3^{i}	1.992 (2)	O1—Zn1—N1	142.89 (9)
Zn1—O1	2.053 (2)	O3^{i}—Zn1—O1W	83.84 (11)
Zn1—N1	2.088 (2)	O1—Zn1—O1W	89.76 (9)
Zn1—O1W	2.202 (3)	N1—Zn1—O1W	90.44 (9)
Zn1—N2^{ii}	2.236 (2)	O3^{i}—Zn1—N2^{ii}	92.57 (9)
O3—Zn1^{iii}	1.992 (2)	O1—Zn1—N2^{ii}	89.77 (9)
N2—Zn1^{iv}	2.236 (2)	N1—Zn1—N2^{ii}	92.57 (9)
O3^{i}—Zn1—O1	119.02 (8)	O1W—Zn1—N2^{ii}	175.60 (10)
O3^{i}—Zn1—N1	97.88 (9)		
		Complex **3**	
Zn1—O3^{i}	1.958 (3)	O3^{i}—Zn1—O1	108.82 (14)
Zn1—O1	1.978 (4)	O3^{i}—Zn1—N1	107.81 (13)
Zn1—N1	2.054 (3)	O1—Zn1—N1	121.32 (15)
Zn1—N2^{ii}	2.066 (4)	O3^{i}—Zn1—N2^{ii}	97.74 (13)
O3—Zn1^{iii}	1.958 (3)	O1—Zn1—N2^{ii}	111.41 (15)
N2—Zn1^{iv}	2.066 (4)	N1—Zn1—N2^{ii}	107.12 (13)
		Complex **4**	
Zn1—O3^{i}	1.9531 (19)	O3^{i}—Zn1—O1	111.15 (8)
Zn1—O1	1.9602 (18)	O3^{i}—Zn1—N2^{ii}	107.34 (8)

Zn1—N2^{ii}	2.045 (2)	O1—Zn1—N2^{ii}	118.68 (8)
Zn1—N1	2.065 (2)	O3^{i}—Zn1—N1	96.53 (8)
O3—Zn1^{iii}	1.9531 (18)	O1—Zn1—N1	112.43 (9)
N2—Zn1^{iv}	2.046 (2)	N2^{ii}—Zn1—N1	108.35 (8)

Symmetry codes, **for 1:** (i) *x*-1/4, -*y*+7/4, *z*+1/4; (ii) -*x*+1/4, *y*-1/4, *z*-1/4; (iii) *x*+1/4, -*y*+7/4, *z*-1/4; (iv) -*x*+1/4, *y*+1/4, *z*+1/4; (v) -*x*, -*y*+2, *z***; for 2:** (i) *x*, -*y*, *z*+1/2; (ii) *x*-1/2, -*y*+1/2, *z*-1/2; (iii) *x*, -*y*, *z*-1/2; (iv) *x*+1/2, -*y*+1/2, *z*+1/2**; for 3:** (i) *x*-1/2, -*y*+1/2, *z*-1/2; (ii) -*x*+3/2, *y*+1/2, -*z*+3/2; (iii) *x*+1/2, -*y*+1/2, *z*+1/2; (iv) -*x*+3/2, *y*-1/2, -*z*+3/2**; for 4:** (i) *x*-1/2, -*y*+1/2, *z*-1/2; (ii) -*x*+5/2, *y*-1/2, -*z*+3/2; (iii) *x*+1/2, -*y*+1/2, *z*+1/2; (iv) -*x*+5/2, *y*+1/2, -*z*+3/2.

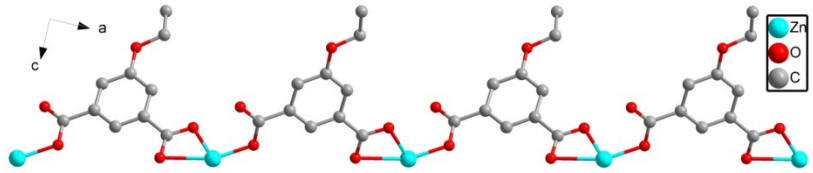


Fig. S1 View of the 1D chains constructed by EtOip and Zn(II) in **1**..

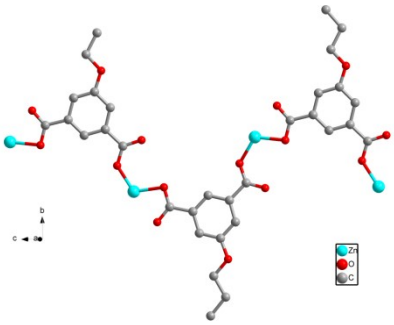


Fig. S2 View of the 1-D chain constructed by PrOip and Zn(II) in **2**.

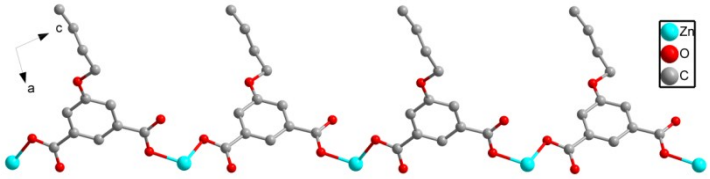


Fig. S3 View of the 1-D chain constructed by ^{n}BuOip and Zn(II) in **3**.

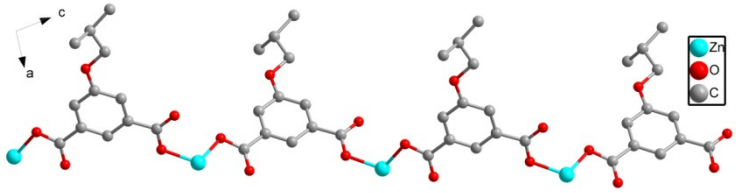


Fig. S4 View of the 1-D chain constructed by ^{i}BuOip and Zn(II) in **4**.

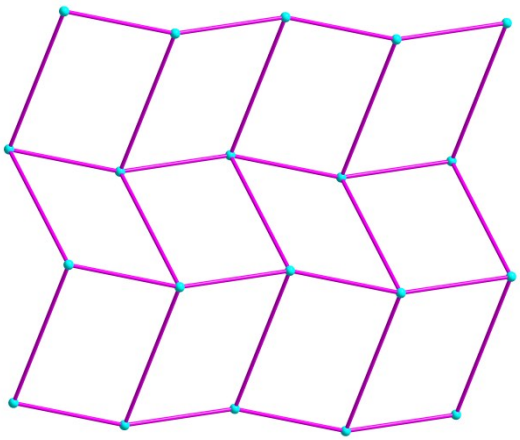


Fig. S5 View of the 4-connected sql/Shubnikov tetragonal plane net with the point symbol $\{4^4 \cdot 6^2\}$ in **3** and **4**.

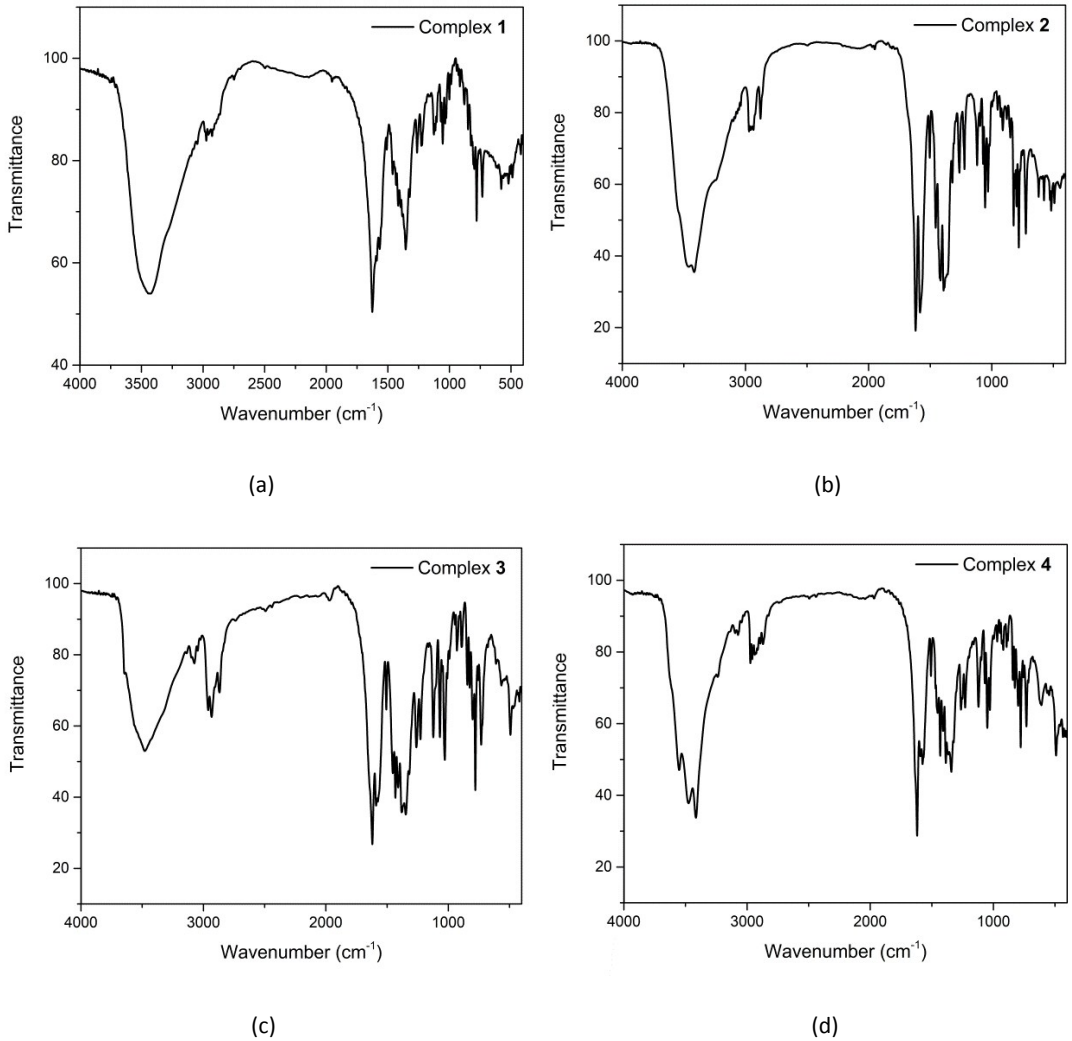


Fig. S6 FT-IR spectrum for **1** (a); **2** (b); **3** (c) and **4** (d).

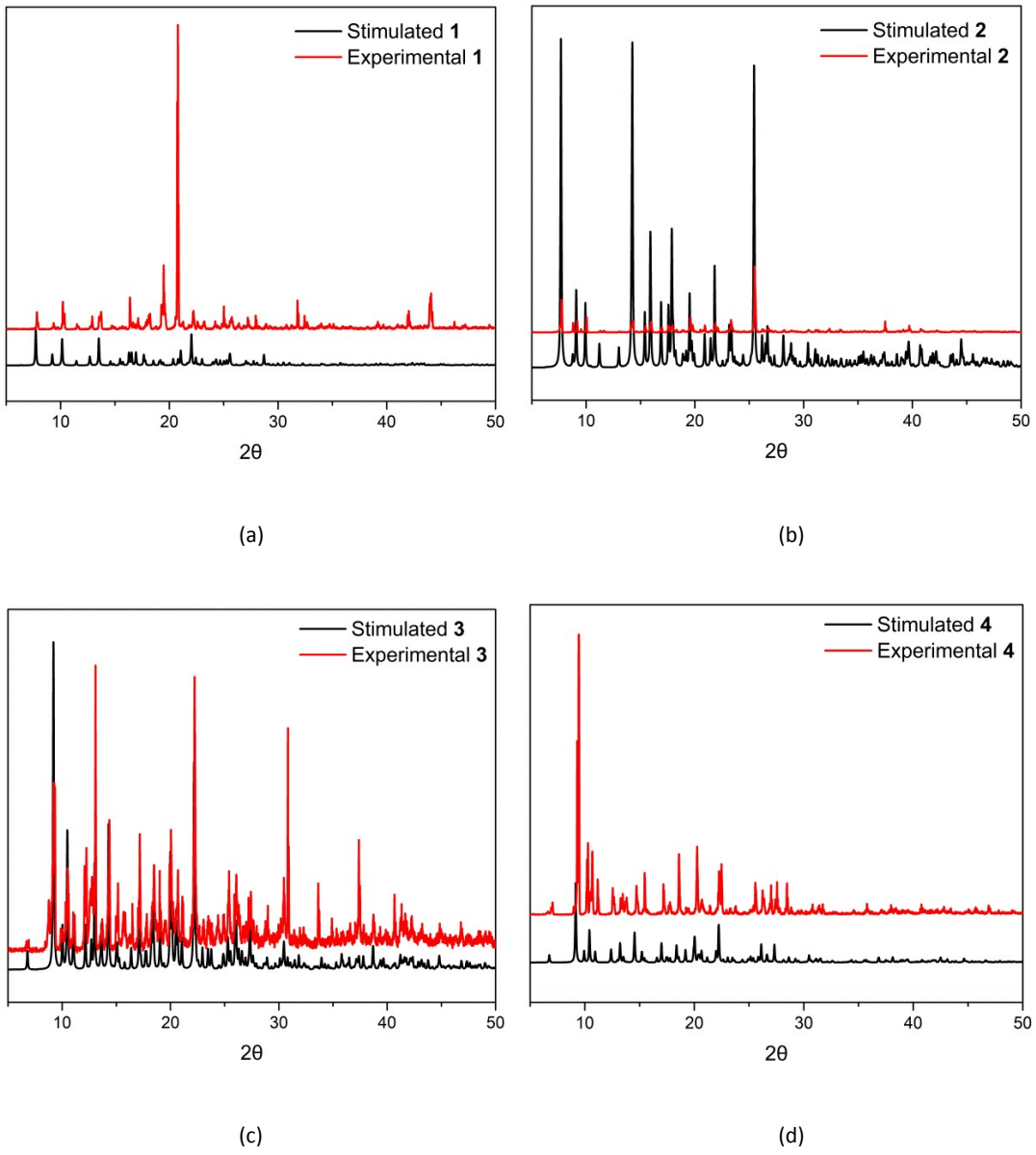
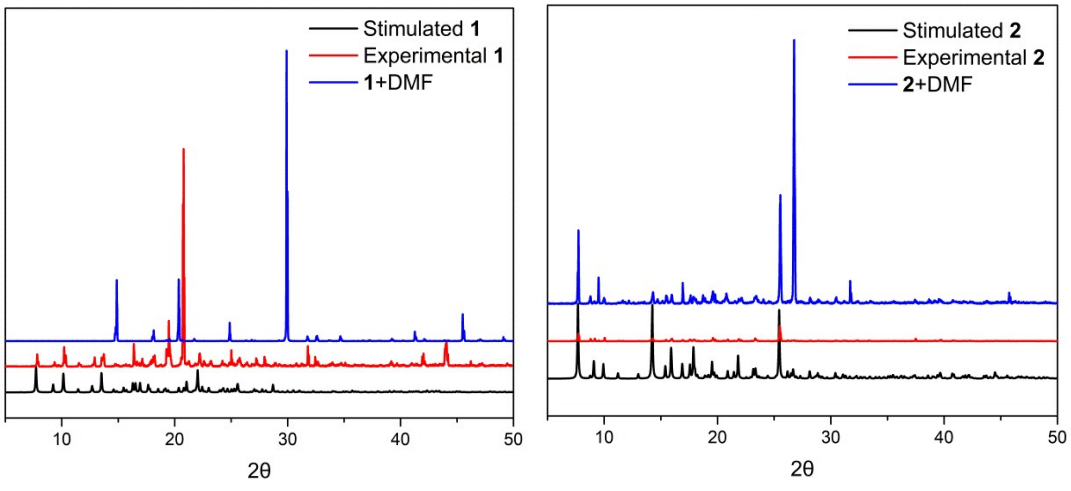
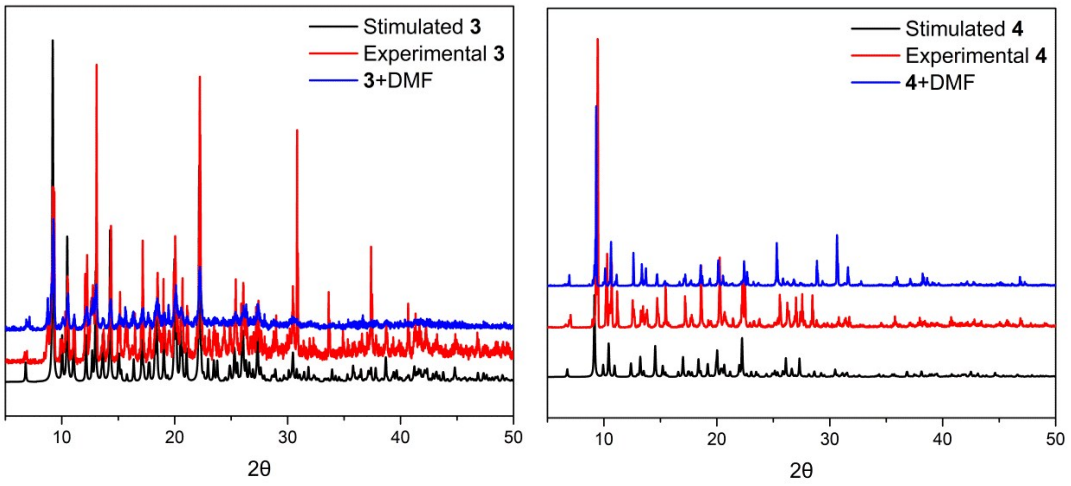


Fig. S7 Powder XRD patterns for **1** (a); **2** (b); **3** (c) and **4**(d). Black: simulated from single crystal analysis and experimental; Red: as synthesized.

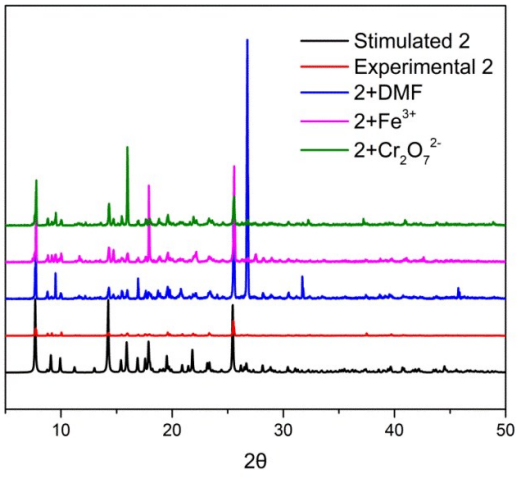


(a) (b)

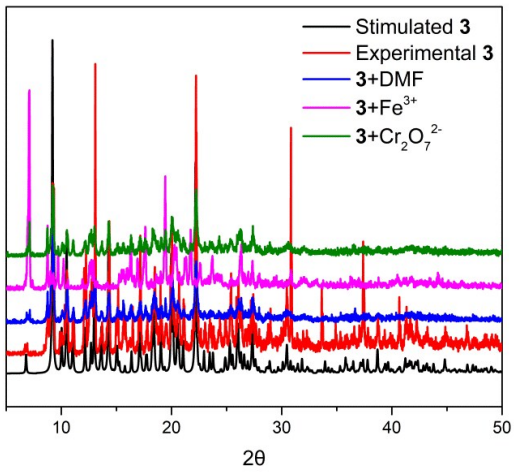


(c) (d)

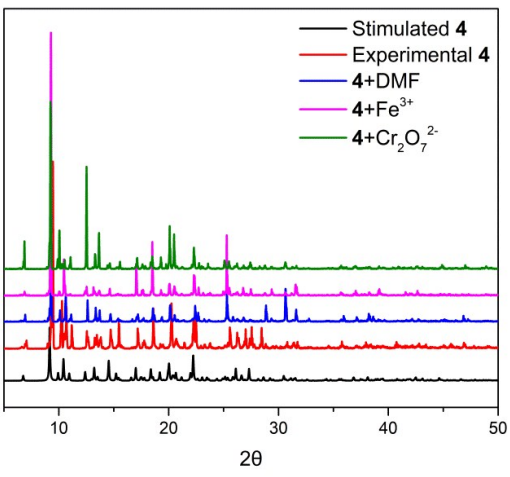
Fig. S8 Powder XRD patterns for **1** (a); **2** (b); **3** (c) and **4** (d). Black: simulated from single crystal analysis and experimental; Red: as synthesized; Blue: complexes in DMF solution.



(a)



(b)



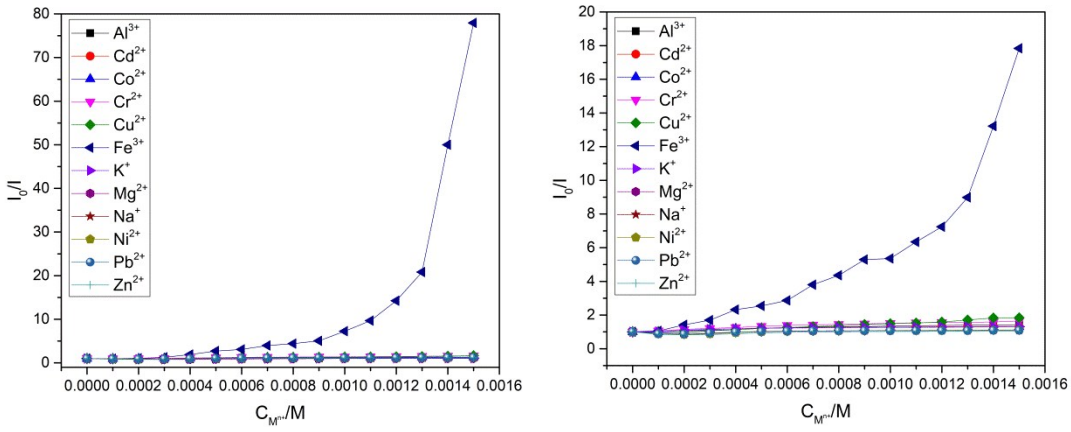
(c)

Fig. S9 PXRD patterns for **2** (a); **3** (b) and **4** (c) after the detection of Fe^{3+} (magenta,) and Cr_2O7^{2-}(green).

Table S2 The values of K_{SV} for Complexes **2-3**.

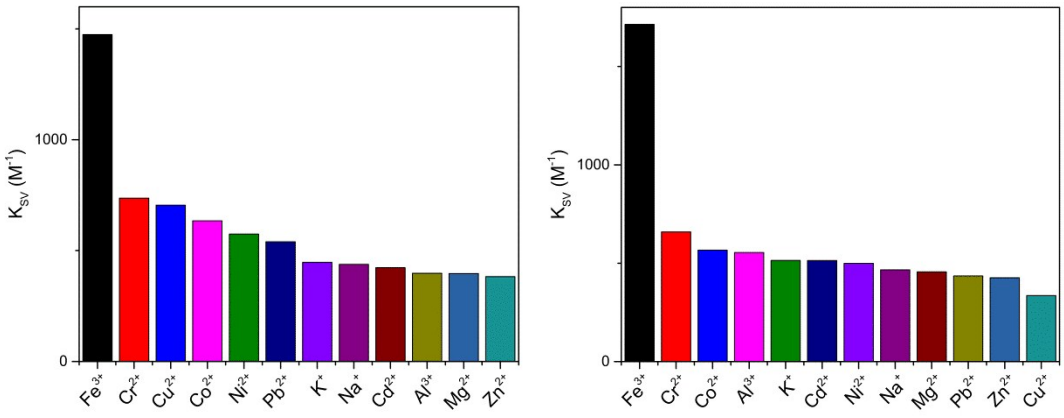
Compound	Ions	Stern−Volmer equation	K_{SV}/M^{-1}	R^2
2	Fe^{3+}	$I_0/I=4404[Fe^{3+}]+0.9381$	4404	0.9911
	Cu^{2+}	$I_0/I=1583[Cu^{2+}]+0.9314$	2388	0.9268
	Ni^{2+}	$I_0/I=1320[Ni^{2+}]+0.6497$	1320	0.9878
	Co^{2+}	$I_0/I=1111[Co^{2+}]+0.6957$	1111	0.9578
	Cr^{2+}	$I_0/I=890.2[Cr^{2+}]+0.8822$	890.2	0.9848
	Pb^{2+}	$I_0/I=574.8[Pb^{2+}]+0.7466$	574.8	0.9880
	Al^{3+}	$I_0/I=521.9[Al^{3+}]+0.7208$	521.9	0.9945
	K^{+}	$I_0/I=464.7[K^{+}]+0.7703$	464.7	0.9816
	Mg^{2+}	$I_0/I=460.9[Mg^{2+}]+0.6711$	460.9	0.9744
	Na^{+}	$I_0/I=447.6[Na^{+}]+0.7358$	447.6	0.9859
	Zn^{2+}	$I_0/I=426.1[Zn^{2+}]+0.7167$	426.1	0.9666
	Cd^{2+}	$I_0/I=422.5[Cd^{2+}]+0.6291$	422.5	0.9864
	$Cr_2O_7^{2-}$	$I_0/I=2237[Cr^2O^{72-}]+1.055$	2237	0.9594
	CrO_4^{2-}	$I_0/I=702.4[CrO_4^{2-}]+0.7963$	702.4	0.9733
	ClO_3^{-}	$I_0/I=514.4[ClO_3^{-}]+0.7809$	514.4	0.9739
	Cl^{-}	$I_0/I=488.7[Cl^{-}]+0.7691$	488.7	0.9729
	NO_3^{-}	$I_0/I=464.7[NO_3^{-}]+0.7703$	464.7	0.9816
	I^{-}	$I_0/I=454.0[I^{-}]+0.7631$	454.0	0.9872
	Br^{-}	$I_0/I=432.9[Br^{-}]+0.8578$	432.9	0.9325
	SCN^{-}	$I_0/I=401.1[SCN^{-}]+0.6383$	401.1	0.9549
3	Fe^{3+}	$I_0/I=1474[Fe^{3+}]+1.053$	1474	0.9696
	Cr^{2+}	$I_0/I=736.8[Cr^{2+}]+0.8316$	736.8	0.9941
	Cu^{2+}	$I_0/I=705.1[Cu^{2+}]+0.7377$	705.1	0.9909
	Co^{2+}	$I_0/I=634.6[Co^{2+}]+0.8309$	634.6	0.9881
	Ni^{2+}	$I_0/I=574.7[Ni^{2+}]+0.7014$	574.7	0.9913
	Pb^{2+}	$I_0/I=539.6[Pb^{2+}]+0.7396$	539.6	0.9918
	K^{+}	$I_0/I=447.1[K^{+}]+0.6882$	447.1	0.9856
	Na^{+}	$I_0/I=438.1[Na^{+}]+0.8223$	438.1	0.9744
	Cd^{2+}	$I_0/I=423.2[Cd^{2+}]+0.7888$	423.2	0.9836
	Al^{3+}	$I_0/I=397.7[Al^{3+}]+0.6636$	397.7	0.9956
	Mg^{2+}	$I_0/I=396.6[Mg^{2+}]+0.6517$	396.6	0.9967
	Zn^{2+}	$I_0/I=382.6[Zn^{2+}]+0.7959$	382.6	0.9860
	$Cr_2O_7^{2-}$	$I_0/I=4512[Cr2O_7^{2-}]+0.9199$	4512	0.9824
	CrO_4^{2-}	$I_0/I=573.1[CrO_4^{2-}]+0.7158$	571.3	0.9919
	I^{-}	$I_0/I=492.2[I^{-}]+0.8409$	492.2	0.9977
	Cl^{-}	$I_0/I=468.1[Cl^{-}]+0.7247$	468.1	0.9954
	ClO_3^{-}	$I_0/I=452.6[ClO_3^{-}]+0.7794$	452.6	0.9949
	NO_3^{-}	$I_0/I=447.1[NO_3^{-}]+0.6882$	447.1	0.9856
	SCN^{-}	$I_0/I=438.6[SCN^{-}]+0.6803$	438.6	0.9946
	Br^{-}	$I_0/I=403.3[Br^{-}]+0.7113$	403.3	0.9958

4	Fe^{3+}	$I_0/I=1714[Fe^{3+}]+0.9604$	1714	0.9907
	Cr^{2+}	$I_0/I=659.3[Cr^{2+}]+1.007$	659.3	0.9881
	Co^{2+}	$I_0/I=566.8[Co^{2+}]+0.9481$	566.8	0.9656
	Al^{3+}	$I_0/I=554.4[Al^{3+}]+0.9081$	554.3	0.9963
	K^{+}	$I_0/I=514.0[K^{+}]+0.9907$	514.0	0.9641
	Cd^{2+}	$I_0/I=513.7[Cd^{2+}]+0.9793$	513.7	0.9794
	Ni^{2+}	$I_0/I=499.2[Ni^{2+}]+0.7460$	499.2	0.9767
	Na^{+}	$I_0/I=466.4[Na^{+}]+0.7875$	466.4	0.9642
	Mg^{2+}	$I_0/I=456.0[Mg^{2+}]+0.7674$	456.0	0.9829
	Pb^{2+}	$I_0/I=435.4[Pb^{2+}]+0.7978$	435.4	0.9464
	Zn^{2+}	$I_0/I=426.0[Zn^{2+}]+0.7240$	426.0	0.9826
	Cu^{2+}	$I_0/I=335.5[Cu^{2+}]+0.9950$	335.5	0.9915
	$Cr_2O_7^{2-}$	$I_0/I=1813[Cr_2O_7^{2-}]+1.039$	1813	0.9635
	CrO_4^{2-}	$I_0/I=688.7[CrO_4^{2-}]+0.8873$	688.7	0.9850
	Br^{-}	$I_0/I=600.1[Br^{-}]+1$	600.1	0.9764
	I^{-}	$I_0/I=551.9[I^{-}]+0.7558$	551.9	0.9898
	SCN^{-}	$I_0/I=550.4[SCN^{-}]+0.8376$	550.4	0.9584
	ClO_3^{-}	$I_0/I=503.5[ClO_3^{-}]+1.017$	503.5	0.9511
	NO_3^{-}	$I_0/I=514.0[NO_3^{-}]+0.9907$	514.0	0.9641
	Cl^{-}	$I_0/I=498.8[Cl^{-}]+0.7110$	498.8	0.9812



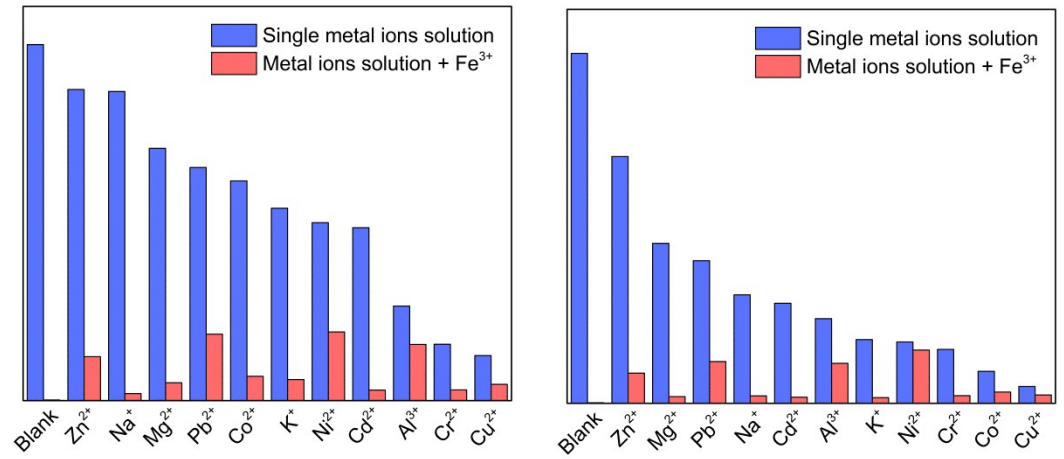
(a) (b)

Fig. S10 I_0/I of **3** (a) and **4** (b) with different metal ions.



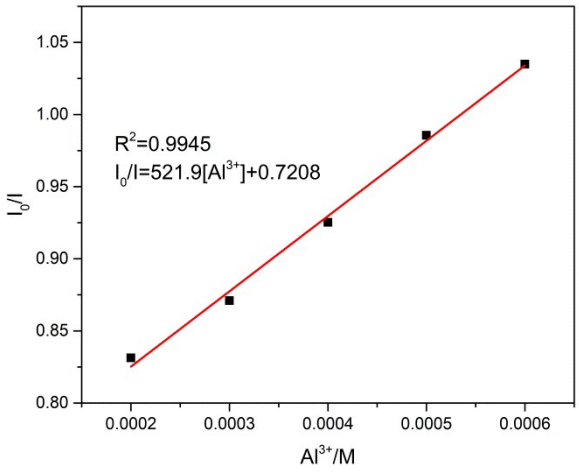
(a) (b)

Fig. S11 K_{SV} of **3** (a) and **4** (b) in DMF solution upon gradual addition of different metal ions (0.01 M) at ambient temperature.

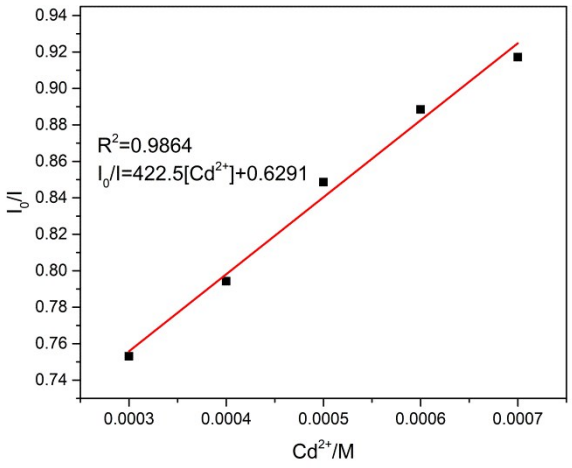


(a) (b)

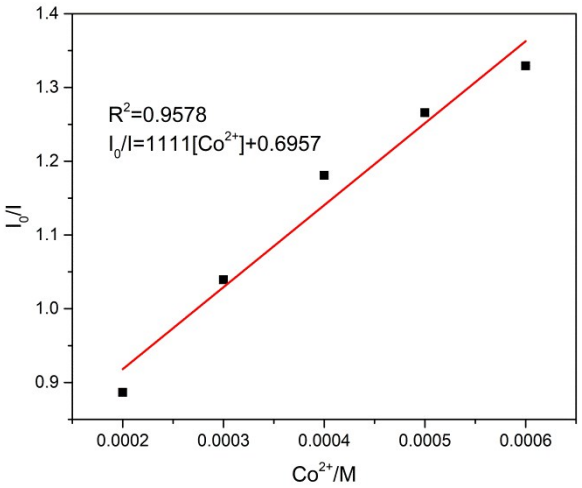
Fig. S12 Luminescence intensities of a suspension of **3**(a) and **4**(b) treated with different metal ions (0.01 M) and luminescence intensities of the suspension of **3**(a) and **4**(b) treated with Fe^{3+} in the presence of other metal ions in DMF.



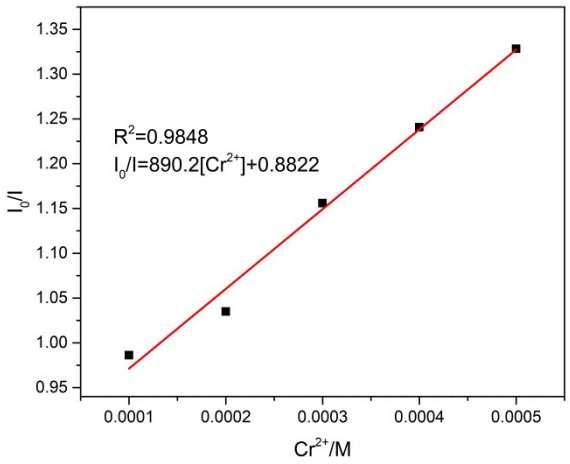
Stern−Volmer equation of **2** at low concentrations of Al^{3+}.



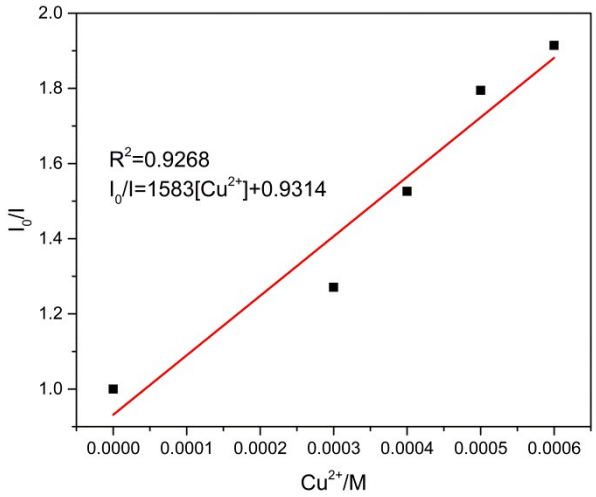
Stern−Volmer equation of **2** at low concentrations of Cd^{2+}.



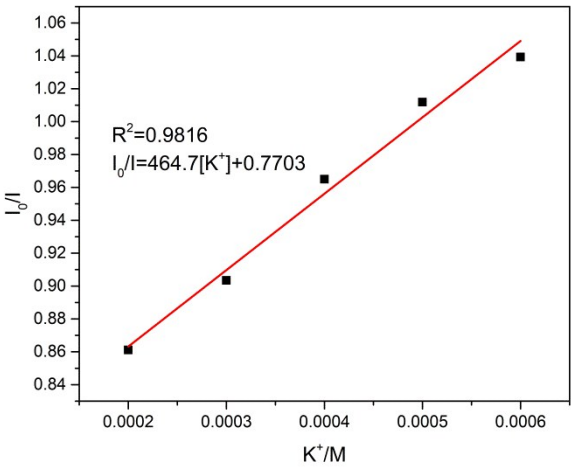
Stern−Volmer equation of **2** at low concentrations of Co^{2+}.



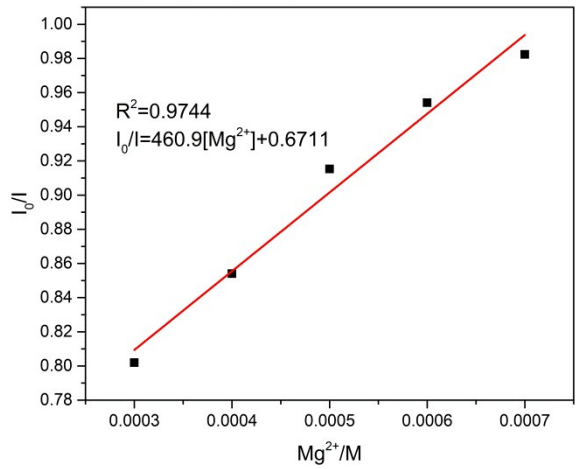
Stern–Volmer equation of **2** at low concentrations of Cr^{2+}.



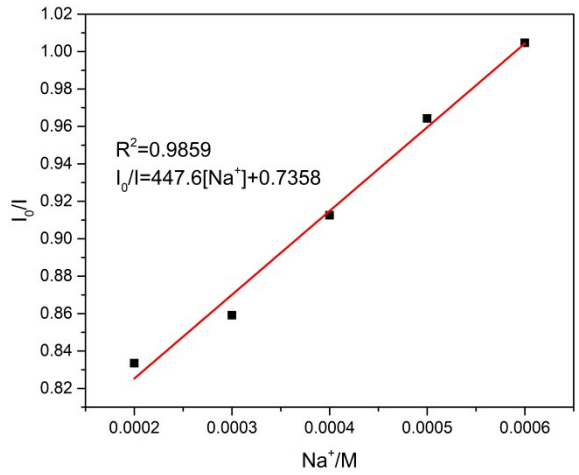
Stern–Volmer equation of **2** at low concentrations of Cu^{2+}.



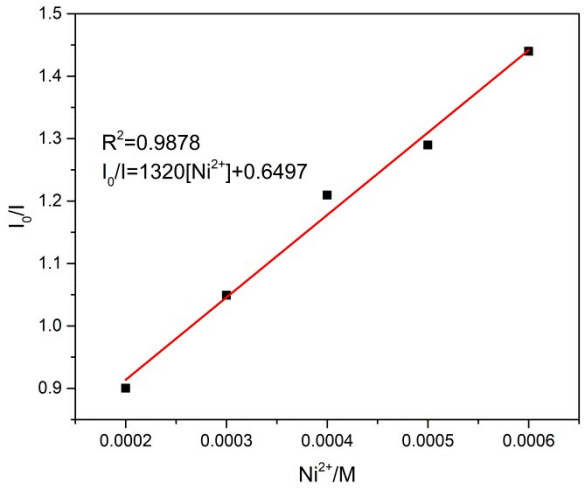
Stern–Volmer equation of **2** at low concentrations of K^{+}.



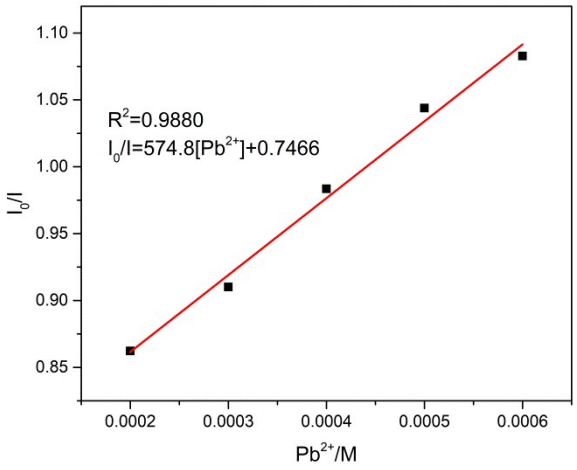
Stern−Volmer equation of **2** at low concentrations of Mg^{2+}.



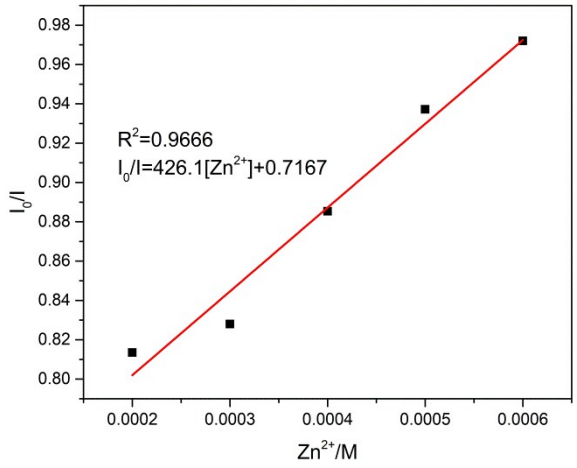
Stern−Volmer equation of **2** at low concentrations of Na^{+}.



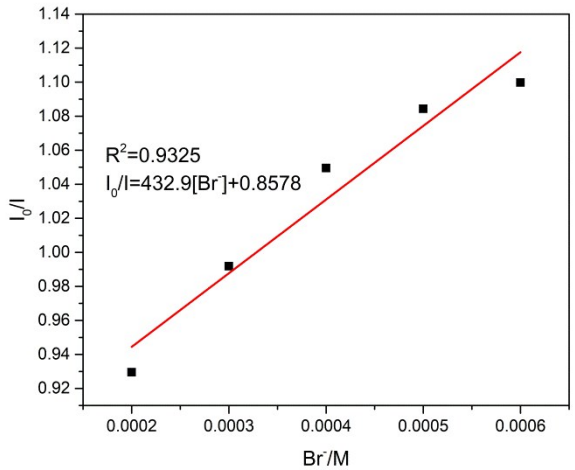
Stern−Volmer equation of **2** at low concentrations of Ni^{2+}.



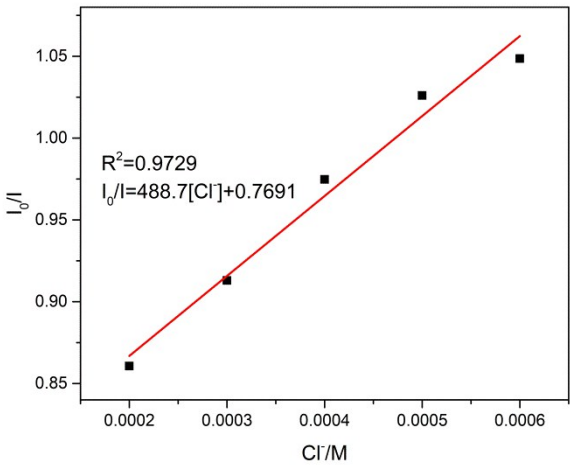
Stern−Volmer equation of **2** at low concentrations of Pb^{2+}.



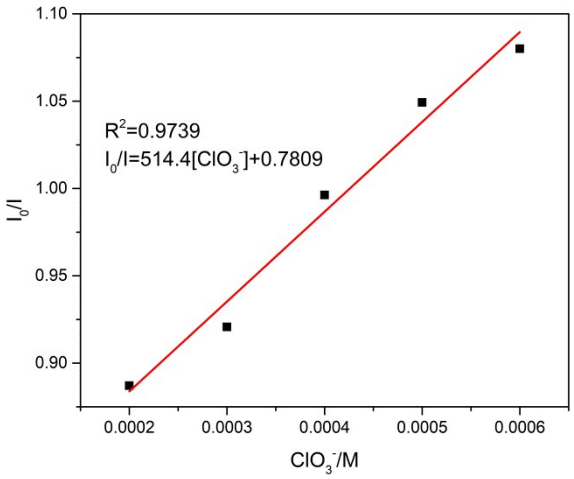
Stern−Volmer equation of **2** at low concentrations of Zn^{2+}.



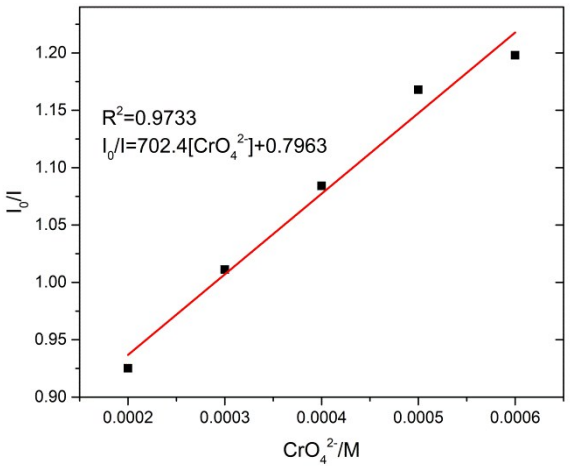
Stern−Volmer equation of **2** at low concentrations of Br^-.



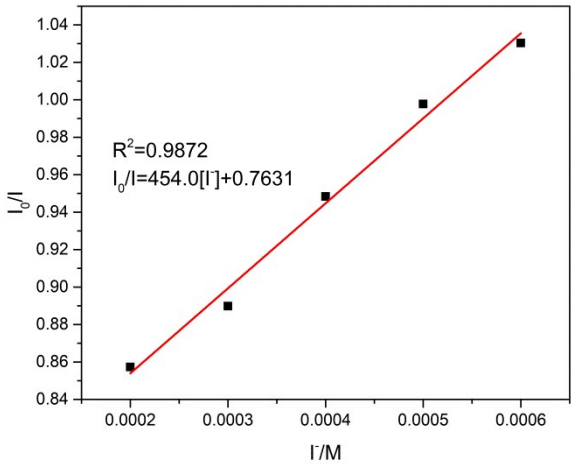
Stern−Volmer equation of **2** at low concentrations of Cl^-.



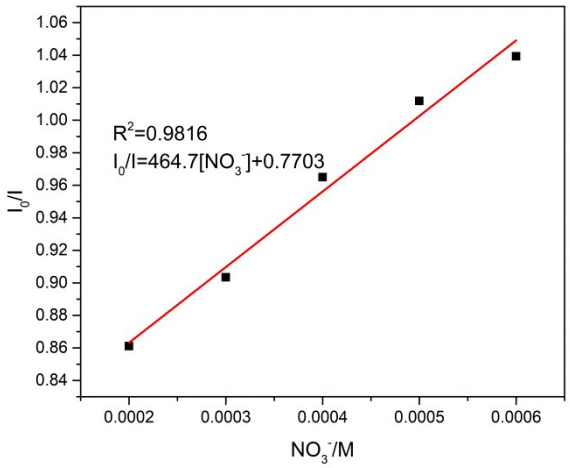
Stern−Volmer equation of **2** at low concentrations of ClO_3^-.



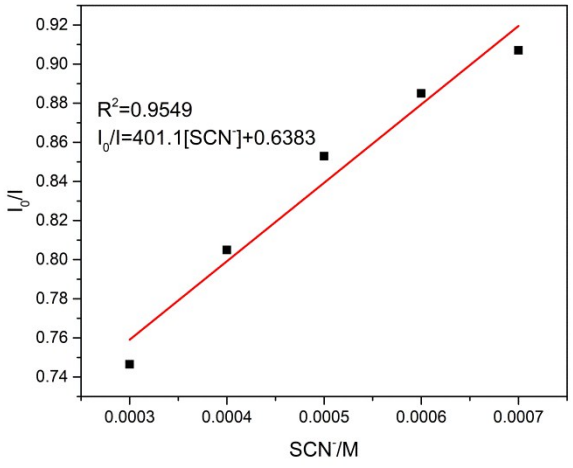
Stern−Volmer equation of **2** at low concentrations of CrO_4^{2-}.



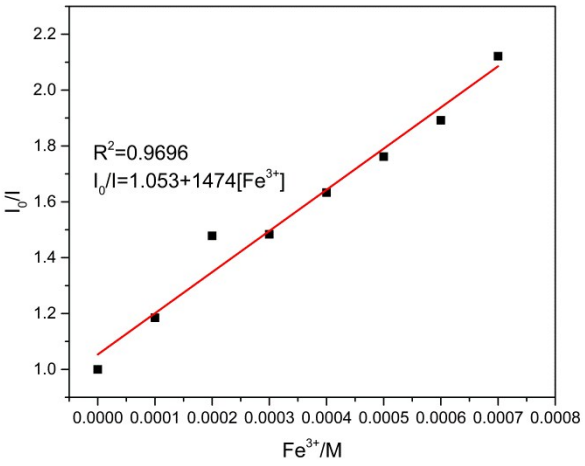
Stern−Volmer equation of **2** at low concentrations of I^-.



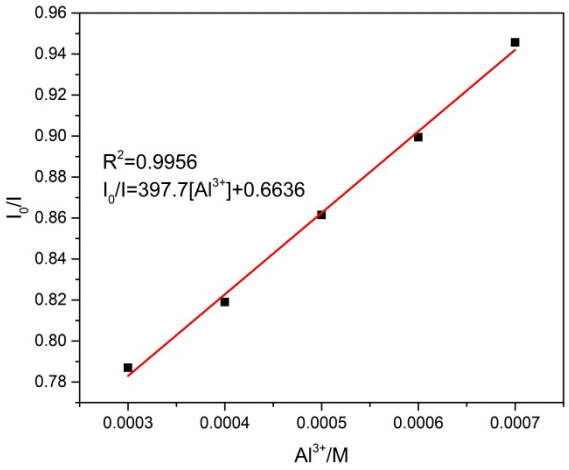
Stern−Volmer equation of **2** at low concentrations of NO_3^-.



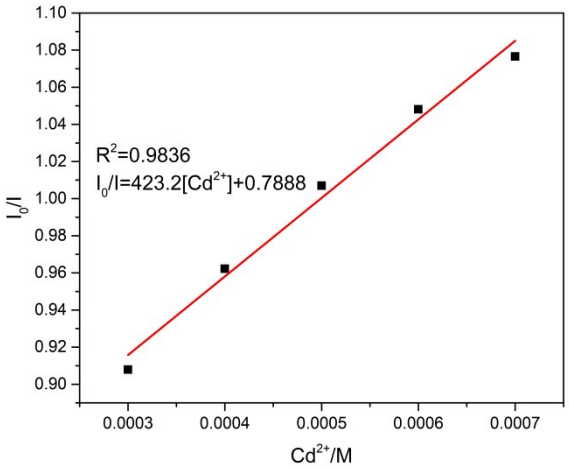
Stern−Volmer equation of **2** at low concentrations of SCN^-.



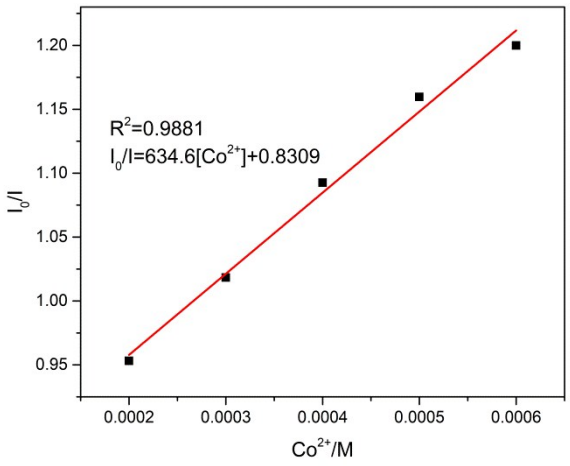
Stern–Volmer equation of **3** at low concentrations of Fe^{3+}.



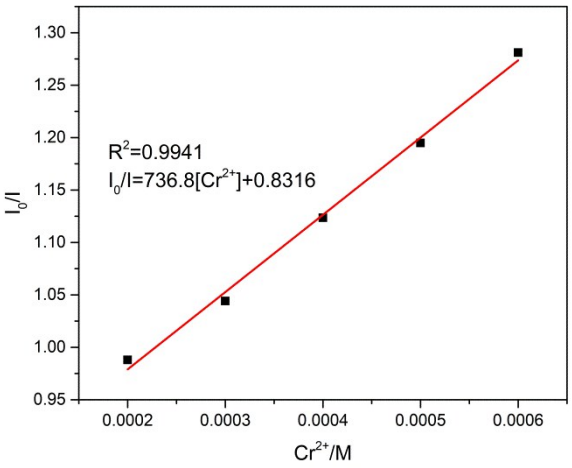
Stern–Volmer equation of **3** at low concentrations of Al^{3+}.



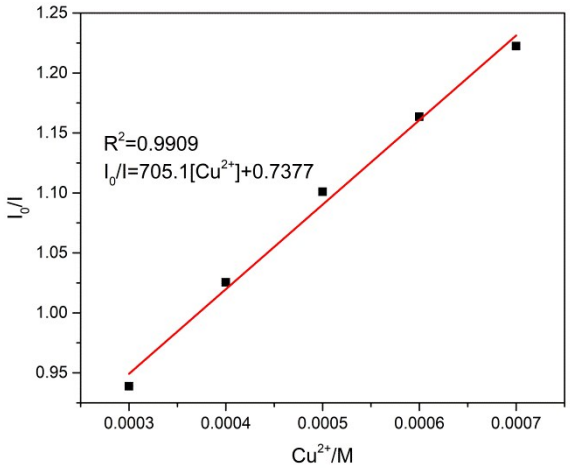
Stern–Volmer equation of **3** at low concentrations of Cd^{2+}.



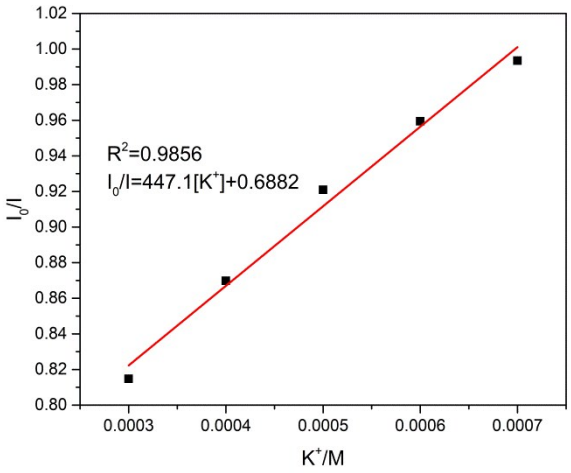
Stern–Volmer equation of **3** at low concentrations of Co^{2+}.



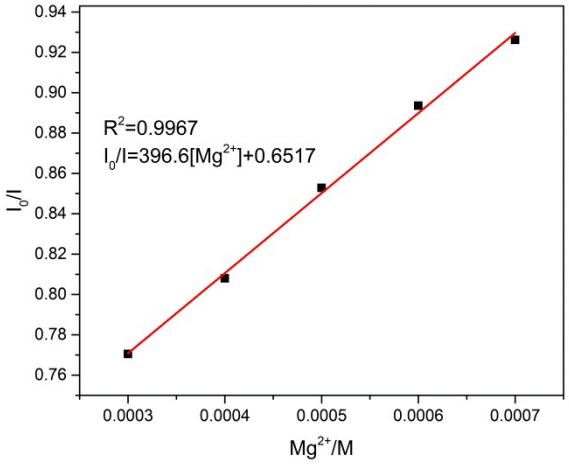
Stern–Volmer equation of **3** at low concentrations of Cr^{2+}.



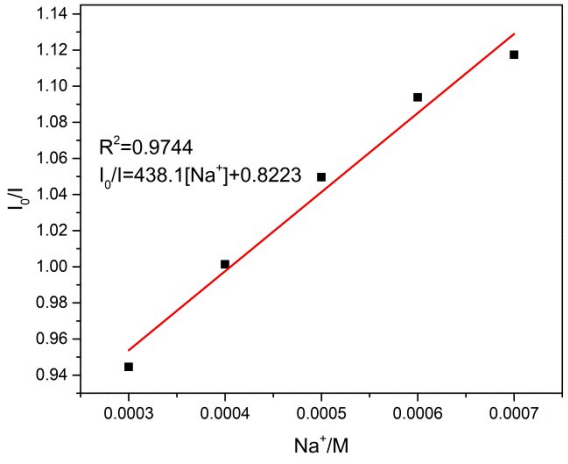
Stern–Volmer equation of **3** at low concentrations of Cu^{2+}.



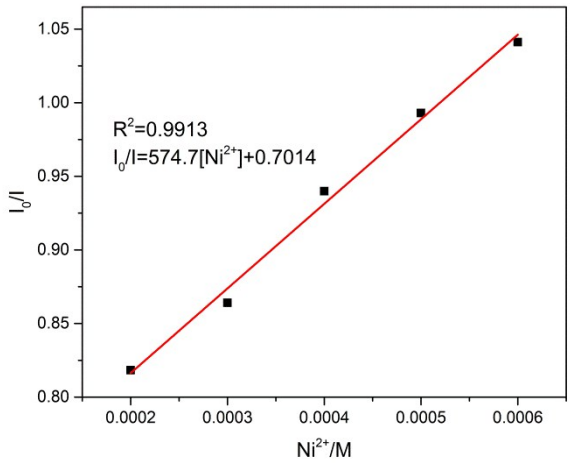
Stern−Volmer equation of **3** at low concentrations of K^+.



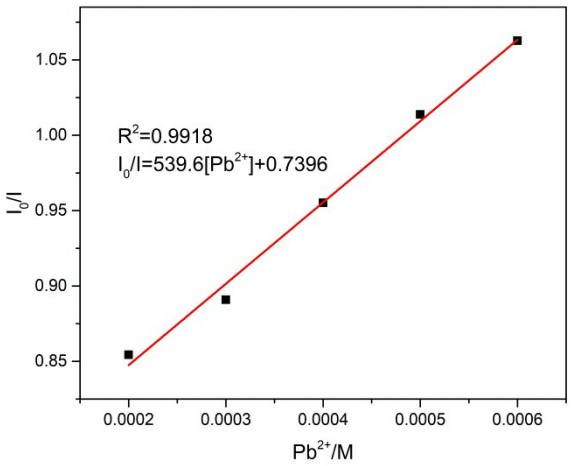
Stern−Volmer equation of **3** at low concentrations of Mg^{2+}.



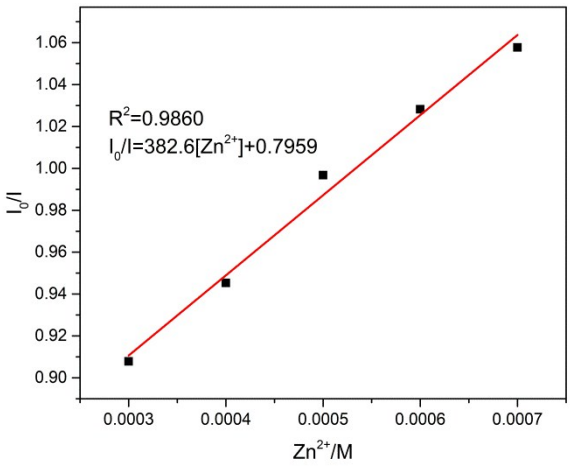
Stern−Volmer equation of **3** at low concentrations of Na^+.



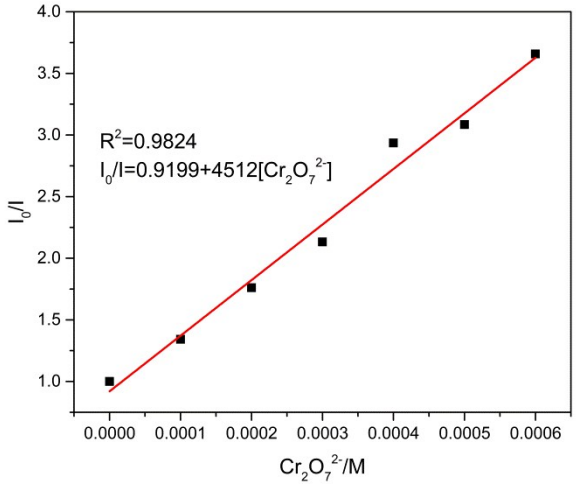
Stern–Volmer equation of **3** at low concentrations of Ni^{2+}.



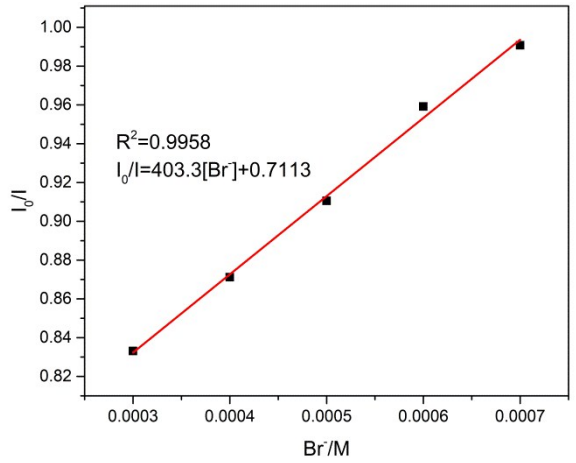
Stern–Volmer equation of **3** at low concentrations of Pb^{2+}.



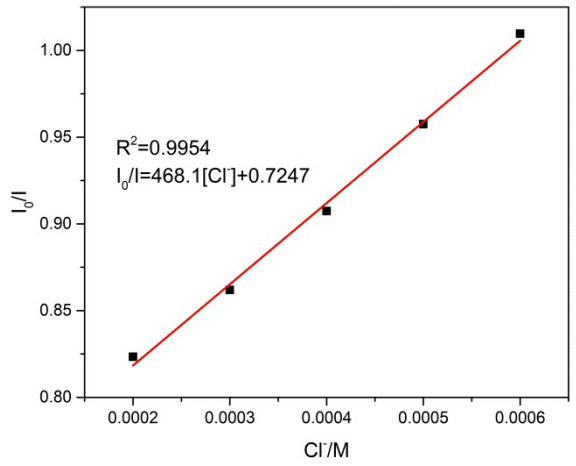
Stern–Volmer equation of **3** at low concentrations of Zn^{2+}.



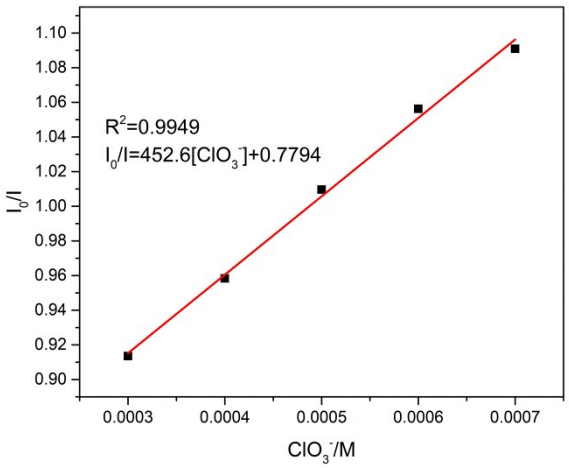
Stern–Volmer equation of **3** at low concentrations of $Cr_2O_7^{2-}$.



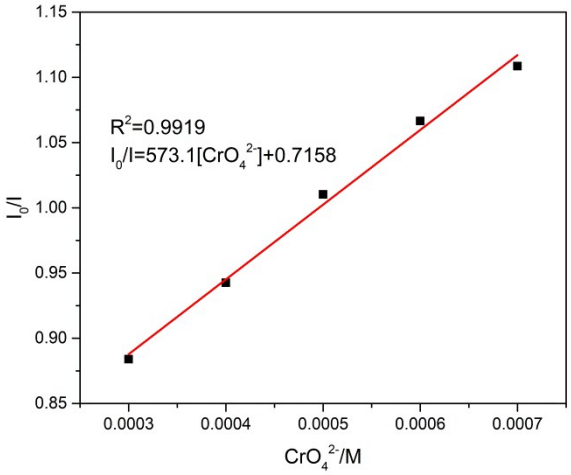
Stern–Volmer equation of **3** at low concentrations of Br^-.



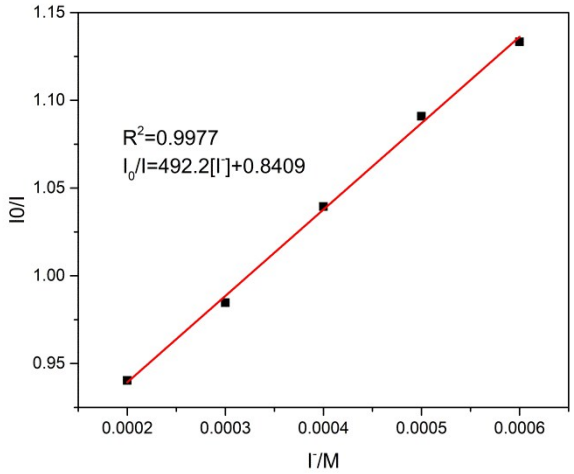
Stern–Volmer equation of **3** at low concentrations of Cl^-.



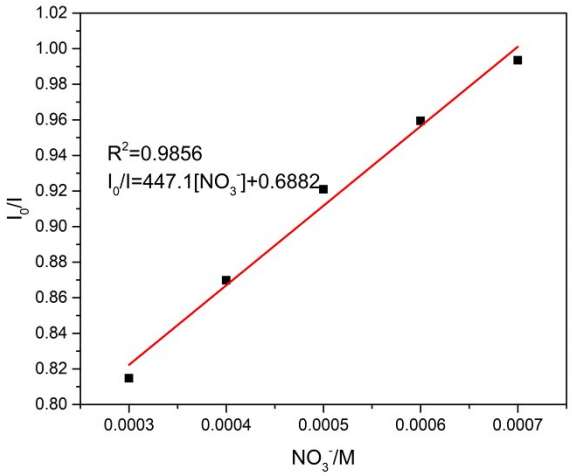
Stern−Volmer equation of **3** at low concentrations of ClO_3^-.



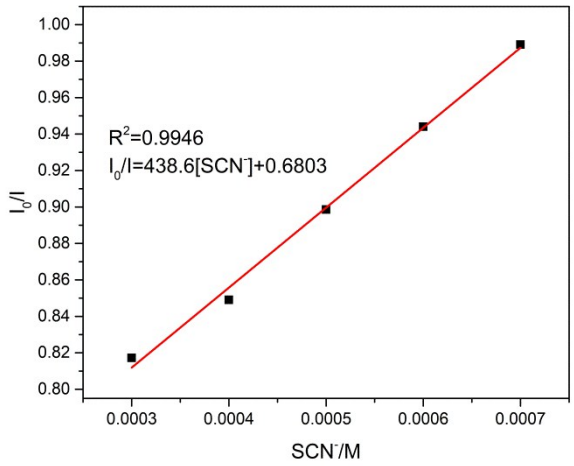
Stern−Volmer equation of **3** at low concentrations of CrO_4^{2-}.



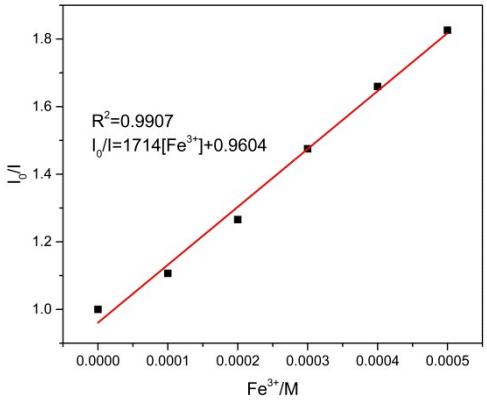
Stern−Volmer equation of **3** at low concentrations of I^-.



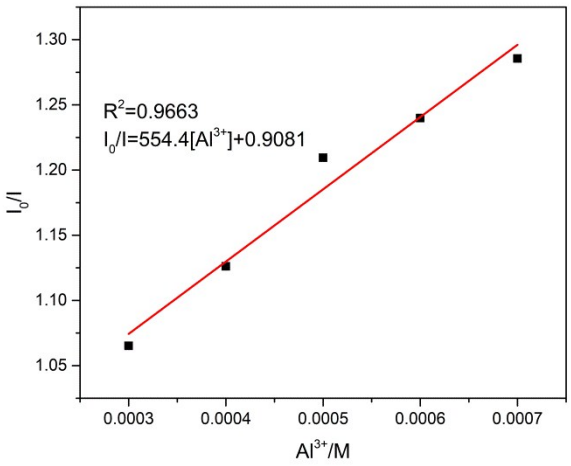
Stern−Volmer equation of **3** at low concentrations of NO_3^-.



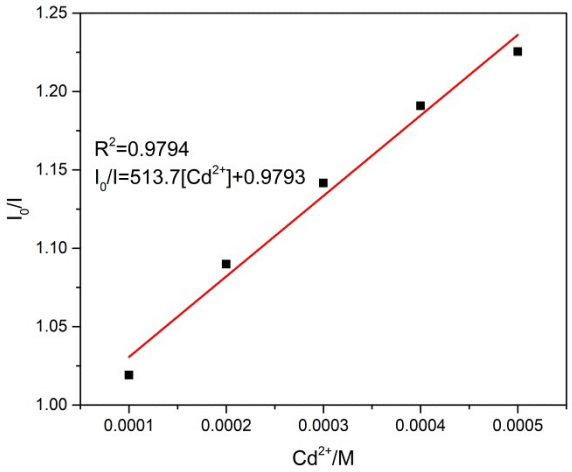
Stern−Volmer equation of **3** at low concentrations of SCN^-.



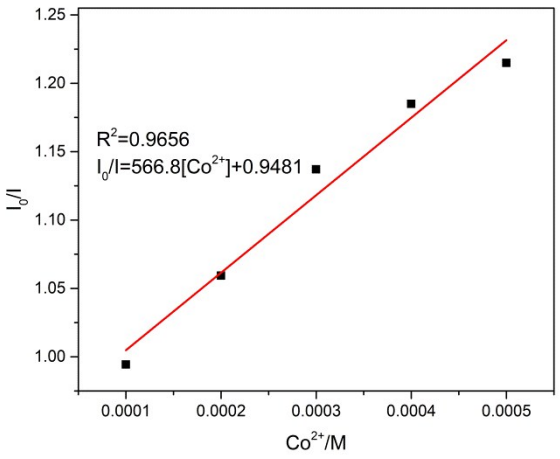
Stern−Volmer equation of **4** at low concentrations of Fe^{3+}.



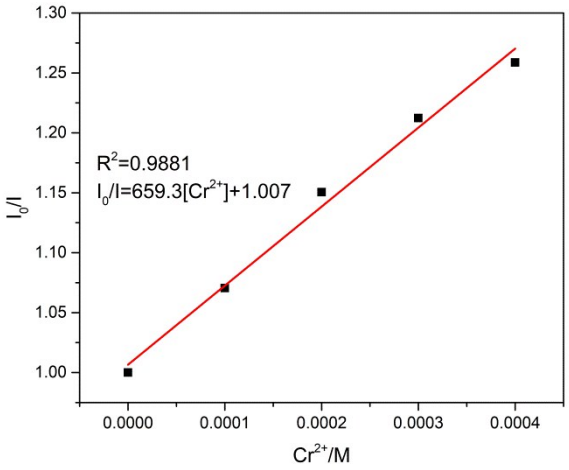
Stern−Volmer equation of **4** at low concentrations of Al^{3+}.



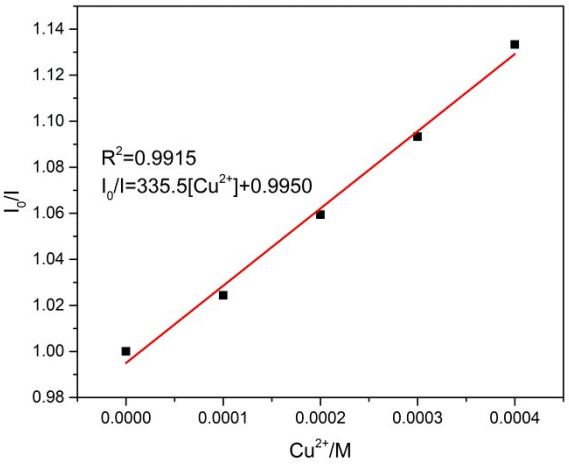
Stern−Volmer equation of **4** at low concentrations of Cd^{2+}.



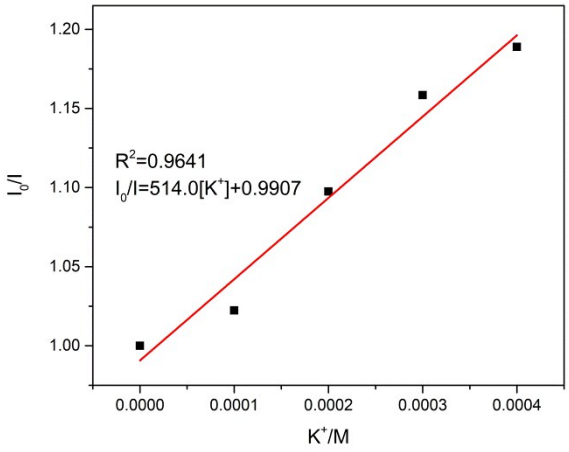
Stern−Volmer equation of **4** at low concentrations of Co^{2+}.



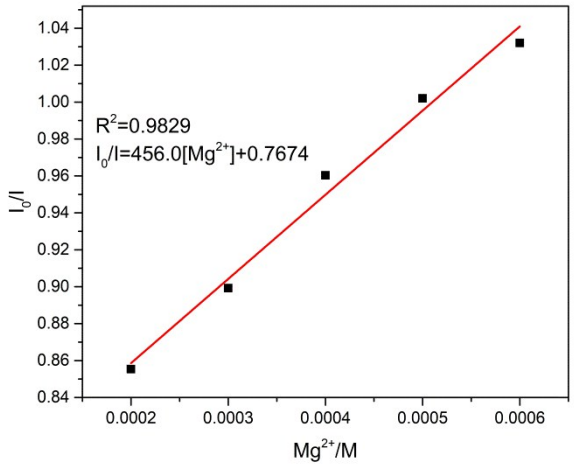
Stern–Volmer equation of **4** at low concentrations of Cr^{2+}.



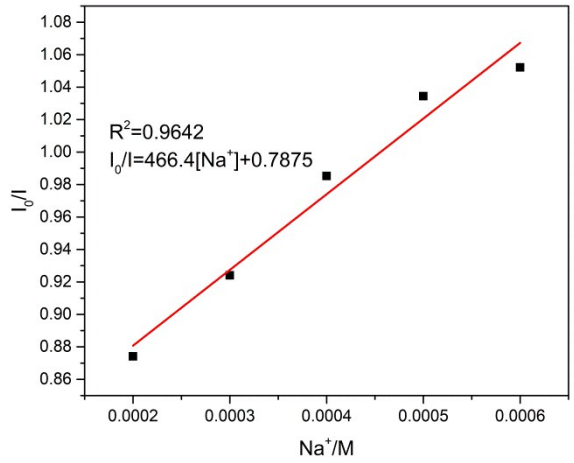
Stern–Volmer equation of **4** at low concentrations of Cu^{2+}.



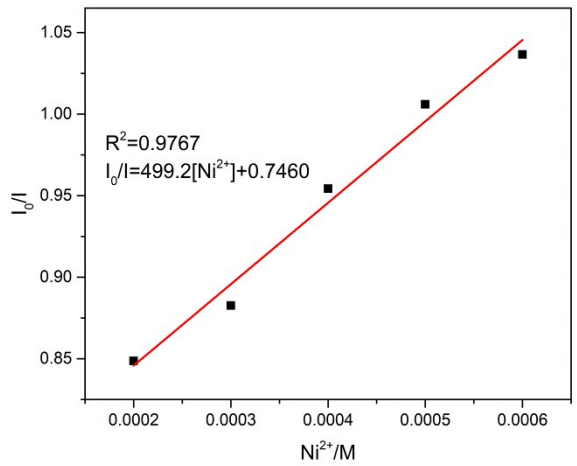
Stern–Volmer equation of **4** at low concentrations of K^+.



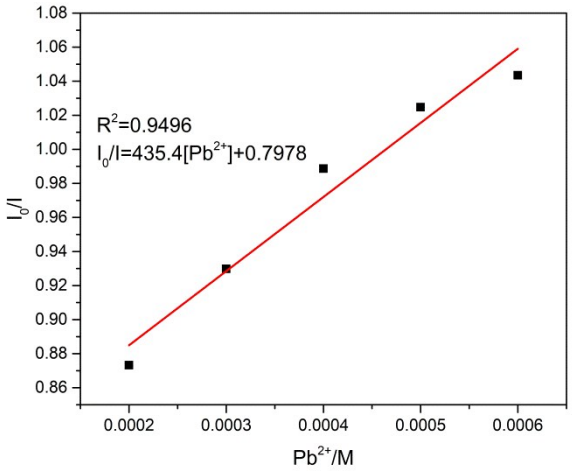
Stern−Volmer equation of **4** at low concentrations of Mg^{2+}.



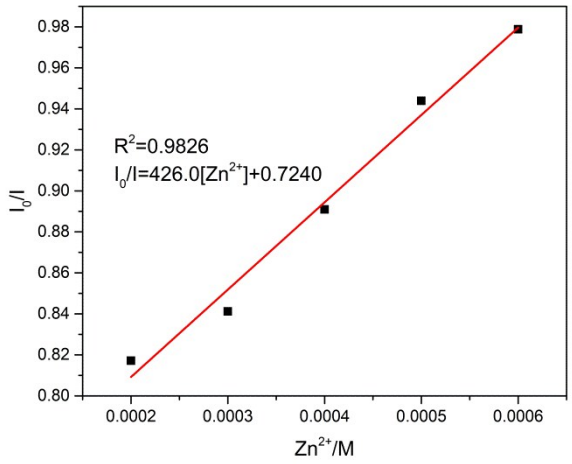
Stern−Volmer equation of **4** at low concentrations of Na^+.



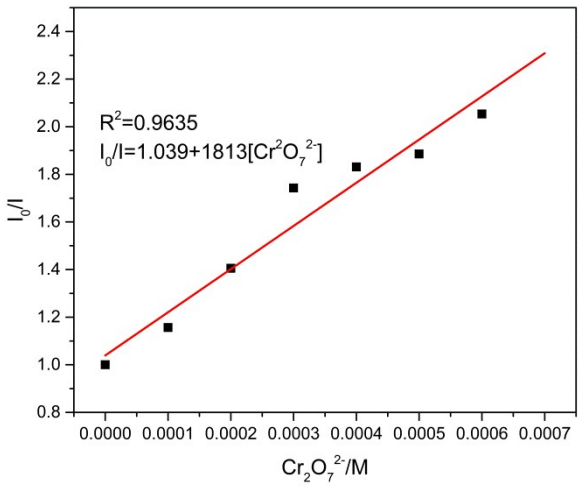
Stern−Volmer equation of **4** at low concentrations of Ni^{2+}.



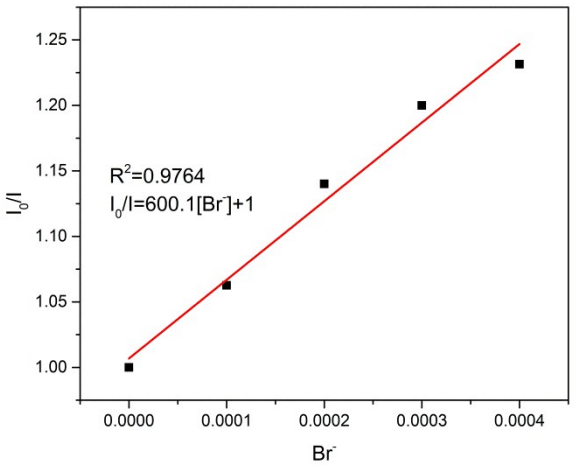
Stern–Volmer equation of **4** at low concentrations of Pb^{2+}.



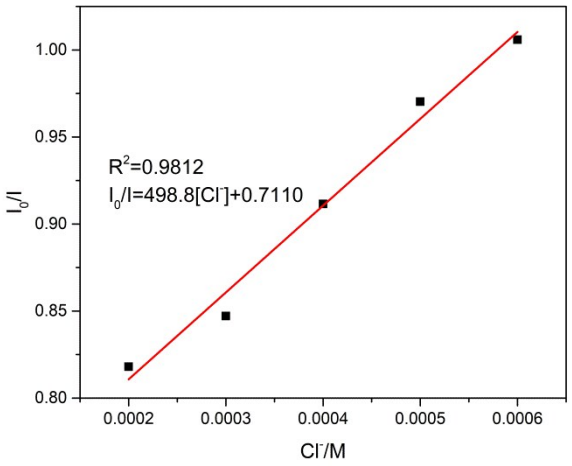
Stern–Volmer equation of **4** at low concentrations of Zn^{2+}.



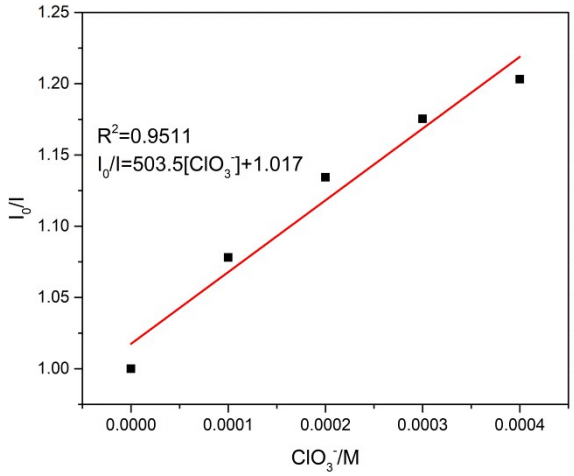
Stern–Volmer equation of **4** at low concentrations of $Cr_2O_7^{2-}$.



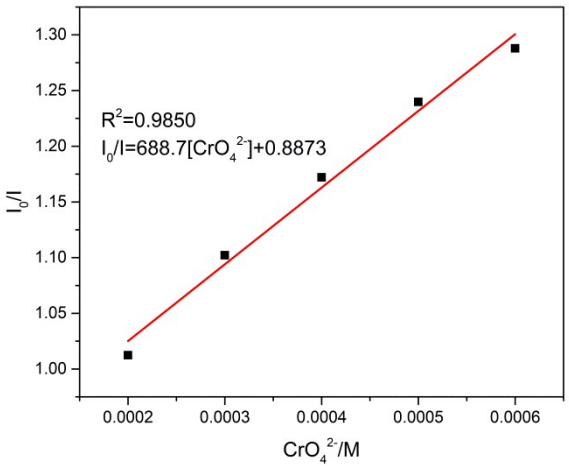
Stern−Volmer equation of **4** at low concentrations of Br^-.



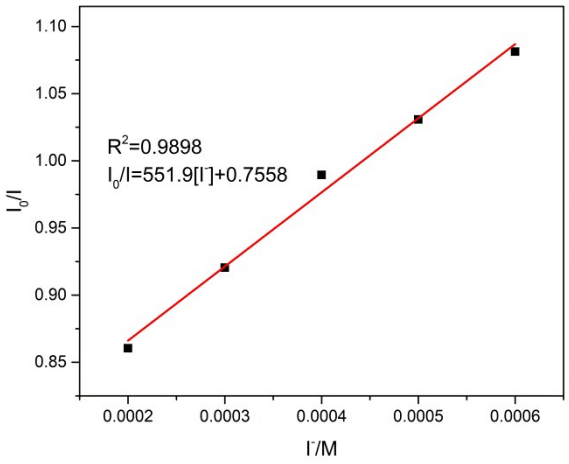
Stern−Volmer equation of **4** at low concentrations of Cl^-.



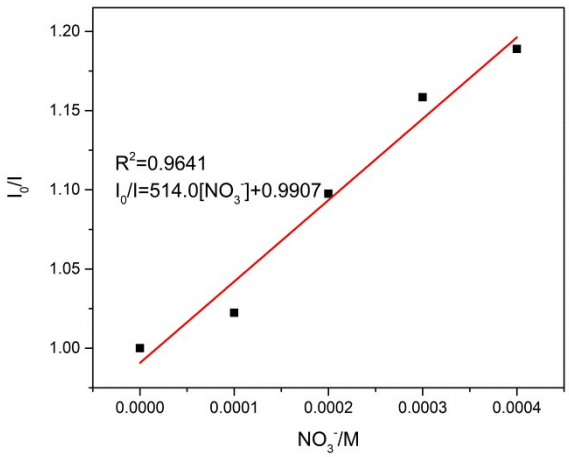
Stern−Volmer equation of **4** at low concentrations of ClO_3^-.



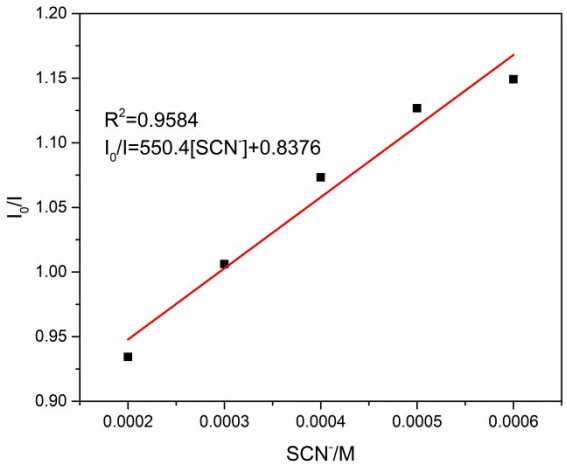
Stern−Volmer equation of **4** at low concentrations of CrO_4^{2-}.



Stern−Volmer equation of **4** at low concentrations of I^-.

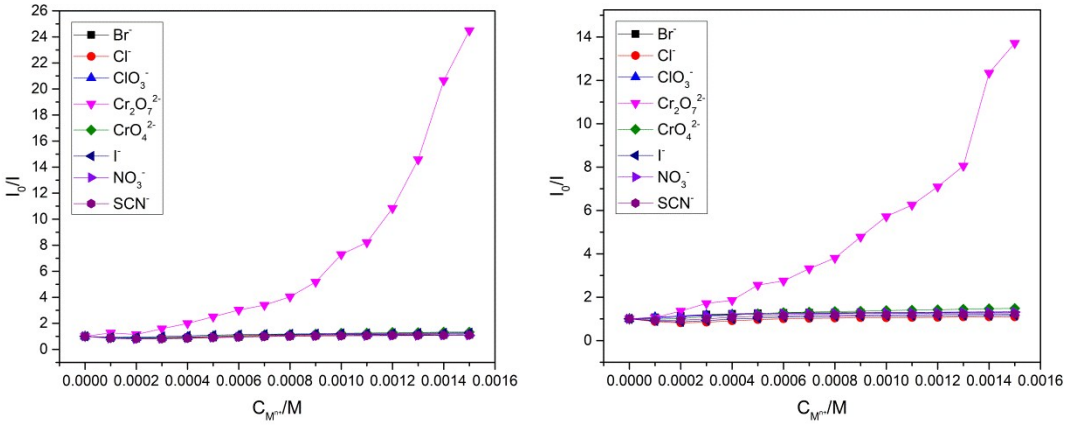


Stern−Volmer equation of **4** at low concentrations of NO_3^-.



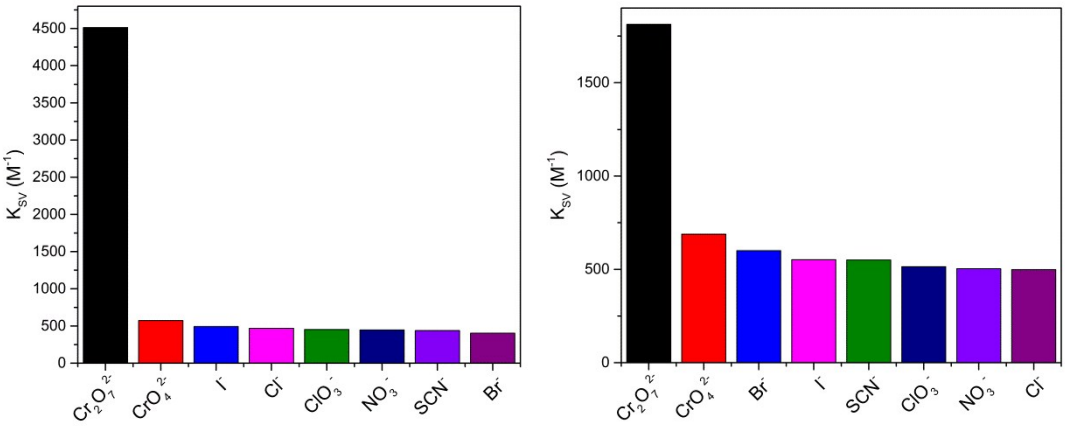
Stern−Volmer equation of **4** at low concentrations of SCN^-.

Fig. S13 Stern−Volmer equation of **3** and **4** at low concentrations.



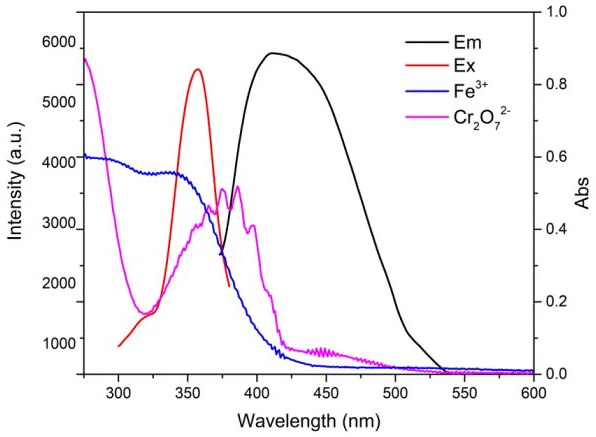
(a) (b)

Fig. S14 I_0/I of **3** (a) and **4** (b) with different anions.

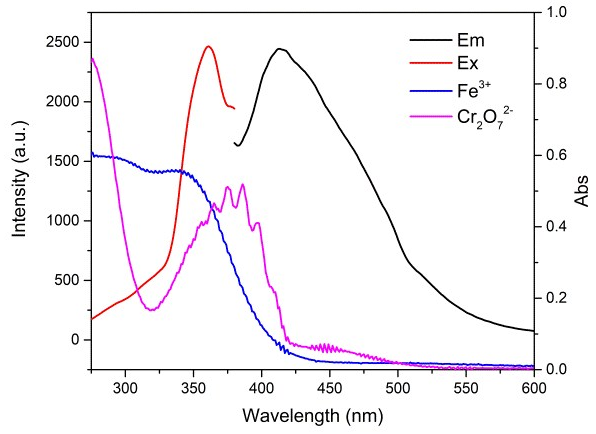


(a) (b)

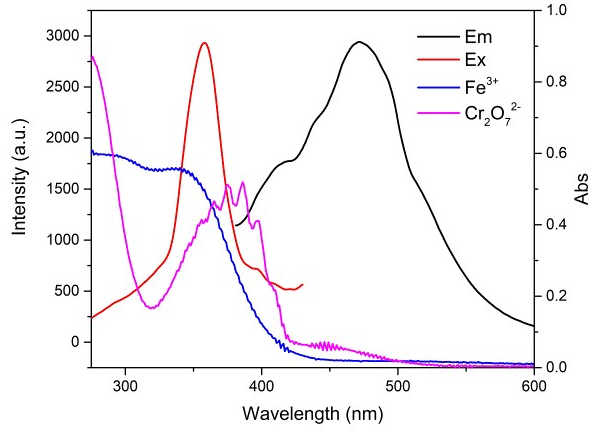
Fig. S15 K_{SV} of **3** (a) and 4 (b) in DMF solution upon gradual addition of different anions (0.01 M) at ambient temperature.



(a)



(b)



(c)

Fig. S16 UV-vis spectra of Fe^{3+} (blue) and $Cr_2O_7^{2-}$ (magenta) in DMF solutions, and the excitation (red) and emission (black) spectra of **2** (a); **3**(b) and **4** (c).