Supporting Information

Assemblies of Cucurbit[6]uril-Based Coordination Complexes with Disulfonate Ligands: From Discrete Complexes to One- and Two-Dimensional Polymers

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Figure S1. PXRD patterns of 1-9.



Figure S2. The TG curves of pure Q[6] and compounds 1 - 9.



Figure S3. The fluorescence emission spectra of 2, 7 and the corresponding sulfonate ligands at solid state.



Figure S4. Fluorescence lifetime of 2 and 7 before and after the addition of Fe^{3+} .



Figure S5. The PXRD patterns of 2 and 7 before and after immersing in the aqueous solution of Fe^{3+} .



Figure S6. Fluorescence quenching and recyclability test for **2** and **7** (initial fluorescence intensity: blue; intensity after quenching: green; inside: complex **7**; outside: complex **2**).



Figure S7. (a) FT-IR spectra of **2** and **7** before and after the addition of Fe^{3+} . (c) Absorption spectra of the solution of Fe^{3+} and emission spectra (normalized) of **2** and **7** suspended stock solution in water.

	1	l			
Ca(1)-O(1)	2.375(4)	Ca(1)-O(1W)	2.483(4)		
Ca(1)-O(4)#1	2.494(4)	Ca(1)-O(2W)	2.427(4)		
Ca(1)-O(6)#2	2.508(4)	Ca(1)-O(3W)	2.670(6)		
Ca(1)-O(7)	2.392(4)	Ca(1)-O(4W)	2.398(4)		
O(1)-Ca(1)-O(7)	104.96(14)	O(7)-Ca(1)-O(4)#1	81.69(13)		
O(1)-Ca(1)-O(4W)	77.73(13)	O(4W)-Ca(1)-O(4)#1	81.26(13)		
O(7)-Ca(1)-O(4W)	151.17(15)	O(2W)-Ca(1)-O(4)#1	69.81(12)		
O(1)-Ca(1)-O(2W)	141.70(13)	O(1W)-Ca(1)-O(4)#1	75.96(13)		
O(7)-Ca(1)-O(2W)	90.42(14)	O(1)-Ca(1)-O(6)#2	78.46(12)		
O(4W)-Ca(1)-O(2W)	105.18(15)	O(7)-Ca(1)-O(6)#2	72.86(12)		
O(1)-Ca(1)-O(1W)	74.00(13)	O(4W)-Ca(1)-O(6)#2	134.57(14)		
O(7)-Ca(1)-O(1W)	74.63(14)	O(2W)-Ca(1)-O(6)#2	72.88(13)		
O(4W)-Ca(1)-O(1W)	78.78(15)	O(1W)-Ca(1)-O(6)#2	129.58(14)		
O(2W)-Ca(1)-O(1W)	144.29(14)	O(4)#1-Ca(1)-O(6)#2	134.17(12)		
O(1)-Ca(1)-O(4)#1	146.04(13)	O(1)-Ca(1)-O(3W)	78.06(16)		
O(1W)-Ca(1)-O(3W)	140.45(17)	O(7)-Ca(1)-O(3W)	140.58(16)		
O(4)#1-Ca(1)-O(3W)	118.01(16)	O(4W)-Ca(1)-O(3W)	68.25(17)		
O(6)#2-Ca(1)-O(3W)	69.30(15)	O(2W)-Ca(1)-O(3W)	68.40(17)		
2					
Sr(1)-O(1)	2.528(3)	Sr(1)-O(1W)	2.623(4)		
Sr(1)-O(2)	2.615(3)	Sr(1)-O(2W)	2.600(4)		
Sr(1)-O(4)#1	2.596(3)	Sr(1)-O(3W)	2.589(3)		
Sr(1)-O(7)	2.531(3)	Sr(1)-O(4W)	2.645(4)		

 Table S1. Selected Bond Lengths (Å) and Angles (°) for 1-9.^a

O(1)-Sr(1)-O(7)	102.36(11)	O(3W)-Sr(1)-O(2)	135.53(10)
O(1)-Sr(1)-O(3W)	75.25(10)	O(4)#1-Sr(1)-O(2)	134.03(9)
O(7)-Sr(1)-O(3W)	147.50(12)	O(2W)-Sr(1)-O(2)	72.28(11)
O(1)-Sr(1)-O(4)#1	147.32(10)	O(1)-Sr(1)-O(1W)	142.61(10)
O(7)-Sr(1)-O(4)#1	80.73(11)	O(7)-Sr(1)-O(1W)	86.43(12)
O(3W)-Sr(1)-O(4)#1	84.92(10)	O(3W)-Sr(1)-O(1W)	115.52(11)
O(1)-Sr(1)-O(2W)	84.26(13)	O(4)#1-Sr(1)-O(1W)	69.59(10)
O(7)-Sr(1)-O(2W)	140.77(12)	O(2W)-Sr(1)-O(1W)	67.60(13)
O(3W)-Sr(1)-O(2W)	71.72(13)	O(2)-Sr(1)-O(1W)	72.35(10)
O(4)#1-Sr(1)-O(2W)	114.10(12)	O(1)-Sr(1)-O(4W)	74.05(11)
O(1)-Sr(1)-O(2)	76.01(10)	O(7)-Sr(1)-O(4W)	73.43(12)
O(7)-Sr(1)-O(2)	72.04(10)	O(3W)-Sr(1)-O(4W)	74.84(12)
O(2)-Sr(1)-O(4W)	127.36(12)	O(4)#1-Sr(1)-O(4W)	75.84(12)
O(1W)-Sr(1)-O(4W)	142.31(11)	O(2W)-Sr(1)-O(4W)	143.78(13)
		3	
Ba(1)-O(1)	2.795(6)	Ba(1)-O(1W)	2.805(5)
Ba(1)-O(2)	2.860(5)	Ba(1)-O(2W)	2.700(6)
Ba(1)-O(4)#2	2.893(5)	Ba(1)-O(3W)	2.815(6)
Ba(1)-O(7)	2.686(5)	Ba(1)-O(4W)	2.838(6)
O(7)-Ba(1)-O(2W)	88.63(18)	O(7)-Ba(1)-O(2)	72.48(16)
O(7)-Ba(1)-O(1)	88.61(17)	O(2W)-Ba(1)-O(2)	71.31(18)
O(2W)-Ba(1)-O(1)	140.84(18)	O(1)-Ba(1)-O(2)	70.64(16)
O(7)-Ba(1)-O(1W)	137.71(16)	O(1W)-Ba(1)-O(2)	65.95(16)
O(2W)-Ba(1)-O(1W)	71.42(18)	O(3W)-Ba(1)-O(2)	123.2(2)
O(1)-Ba(1)-O(1W)	84.94(17)	O(4W)-Ba(1)-O(2)	124.63(17)

O(7)-Ba(1)-O(3W)	67.21(18)	O(7)-Ba(1)-O(1W)#1	140.82(17)
O(2W)-Ba(1)-O(3W)	142.16(19)	O(2W)-Ba(1)-O(1W)#1	65.60(18)
O(1)-Ba(1)-O(3W)	70.11(19)	O(1)-Ba(1)-O(1W)#1	130.12(16)
O(1W)-Ba(1)-O(3W)	145.41(18)	O(1W)-Ba(1)-O(1W)#1	63.27(18)
O(7)-Ba(1)-O(4W)	135.89(17)	O(3W)-Ba(1)-O(1W)#1	115.7(2)
O(2W)-Ba(1)-O(4W)	134.07(18)	O(4W)-Ba(1)-O(1W)#1	70.42(17)
O(1)-Ba(1)-O(4W)	65.69(16)	O(2)-Ba(1)-O(1W)#1	120.90(16)
O(1W)-Ba(1)-O(4W)	77.72(17)	O(7)-Ba(1)-O(4)#2	76.32(17)
O(3W)-Ba(1)-O(4W)	70.41(18)	O(2W)-Ba(1)-O(4)#2	77.20(17)
O(4W)-Ba(1)-O(4)#2	99.77(16)	O(1)-Ba(1)-O(4)#2	139.36(16)
O(2)-Ba(1)-O(4)#2	135.59(16)	O(1W)-Ba(1)-O(4)#2	130.87(16)
O(1W)#1-Ba(1)-			
O(4)#2	69.71(15)	O(3W)-Ba(1)-O(4)#2	69.25(19)
		4	
Ca(1)-O(1)#1	2.437(2)	Ca(1)-O(2W)	2.395(3)
Ca(1)-O(3)#2	2.453(2)	Ca(1)-O(3W)	2.504(3)
Ca(1)-O(4)	2.401(2)	Ca(1)-O(4W)	2.382(3)
Ca(1)-O(1W)	2.447(3)	Ca(1)-O(5W)	2.677(4)
O(4W)-Ca(1)-O(2W)	151.37(12)	O(4)-Ca(1)-O(3)#2	81.40(8)
O(4W)-Ca(1)-O(4)	77.15(10)	O(1)#1-Ca(1)-O(3)#2	132.93(8)
O(2W)-Ca(1)-O(4)	102.83(9)	O(1W)-Ca(1)-O(3)#2	72.71(8)
O(4W)-Ca(1)-O(1)#1	80.80(10)	O(4W)-Ca(1)-O(3W)	77.56(12)
O(2W)-Ca(1)-O(1)#1	84.01(9)	O(2W)-Ca(1)-O(3W)	75.43(9)
O(4)-Ca(1)-O(1)#1	144.60(8)	O(4)-Ca(1)-O(3W)	71.62(8)
O(4W)-Ca(1)-O(1W)	103.27(11)	O(1)#1-Ca(1)-O(3W)	76.84(8)

O(2W)-Ca(1)-O(1W)	93.45(10)	O(1W)-Ca(1)-O(3W)	144.66(9)
O(4)-Ca(1)-O(1W)	143.58(8)	O(3)#2-Ca(1)-O(3W)	131.68(9)
O(1)#1-Ca(1)-O(1W)	68.60(8)	O(4W)-Ca(1)-O(5W)	66.84(14)
O(4W)-Ca(1)-O(3)#2	134.55(11)	O(2W)-Ca(1)-O(5W)	141.78(12)
O(2W)-Ca(1)-O(3)#2	72.48(9)	O(4)-Ca(1)-O(5W)	80.94(12)
O(3)#2-Ca(1)-O(5W)	70.54(11)	O(1)#1-Ca(1)-O(5W)	115.01(12)
O(3W)-Ca(1)-O(5W)	138.99(11)	O(1W)-Ca(1)-O(5W)	66.65(11)
		5	
Sr(1)-O(1)	2.538(3)	Sr(1)-O(2W)	2.717(5)
Sr(1)-O(4)#2	2.595(3)	Sr(1)-O(3W)	2.578(4)
Sr(1)-O(6)#1	2.590(3)	Sr(1)-O(4W)	2.554(4)
Sr(1)-O(1W)	2.544(4)	Sr(1)-O(5W)	2.628(4)
O(1)-Sr(1)-O(1W)	77.23(11)	O(1)-Sr(1)-O(5W)	73.05(13)
O(1)-Sr(1)-O(4W)	101.61(14)	O(1W)-Sr(1)-O(5W)	76.45(15)
O(1W)-Sr(1)-O(4W)	149.76(16)	O(4W)-Sr(1)-O(5W)	74.42(15)
O(1)-Sr(1)-O(3W)	143.82(12)	O(3W)-Sr(1)-O(5W)	142.90(14)
O(1W)-Sr(1)-O(3W)	109.55(15)	O(6)#1-Sr(1)-O(5W)	131.12(13)
O(4W)-Sr(1)-O(3W)	89.37(17)	O(4)#2-Sr(1)-O(5W)	76.15(13)
O(1)-Sr(1)-O(6)#1	79.87(10)	O(1)-Sr(1)-O(2W)	84.16(15)
O(1W)-Sr(1)-O(6)#1	135.56(12)	O(1W)-Sr(1)-O(2W)	68.53(15)
O(4W)-Sr(1)-O(6)#1	72.20(13)	O(4W)-Sr(1)-O(2W)	141.71(15)
O(3W)-Sr(1)-O(6)#1	70.81(13)	O(3W)-Sr(1)-O(2W)	67.05(16)
O(1)-Sr(1)-O(4)#2	145.23(10)	O(6)#1-Sr(1)-O(2W)	71.68(13)
O(1W)-Sr(1)-O(4)#2	80.27(11)	O(4)#2-Sr(1)-O(2W)	111.64(15)
O(4W)-Sr(1)-O(4)#2	85.06(13)	O(5W)-Sr(1)-O(2W)	141.63(15)

	6)		
Ba(1)-O(1)	2.770(3)	Ba(2)-O(19)	2.788(4)	•
Ba(1)-O(2)	2.746(3)	Ba(1)-O(1W)	3.018(5)	
Ba(1)-O(4)#1	2.788(3)	Ba(1)-O(2W)	2.846(3)	
Ba(1)-O(5)#1	2.759(3)	Ba(2)-O(3W)	2.944(5)	
Ba(2)-O(7)	2.661(4)	Ba(2)-O(4W)	2.757(4)	
Ba(2)-O(8)	2.778(3)	Ba(2)-O(5W)	2.795(6)	
Ba(1)-O(13)	2.771(3)	Ba(2)-O(6W)	2.704(4)	
Ba(2)-O(10)#2	2.766(3)	Ba(1)-O(7W)	2.882(9)	
O(2)-Ba(1)-O(1)	75.68(11)	O(6W)-Ba(2)-O(8)	68.61(12)	
O(4W)-Ba(2)-O(8)	143.25(13)	O(7)-Ba(2)-O(6W)	140.42(12)	
O(2)-Ba(1)-O(5)#1	152.31(10)	O(10)#2-Ba(2)-O(8)	129.25(10)	
O(5)#1-Ba(1)-O(1)	89.53(10)	O(7)-Ba(2)-O(19)	86.61(13)	
O(2)-Ba(1)-O(13)	73.09(10)	O(6W)-Ba(2)-O(19)	88.09(14)	
O(5)#1-Ba(1)-O(13)	80.86(10)	O(4W)-Ba(2)-O(19)	144.09(14)	
O(1)-Ba(1)-O(13)	76.69(10)	O(10)#2-Ba(2)-O(19)	81.16(12)	
O(2)-Ba(1)-O(4)#1	104.84(11)	O(8)-Ba(2)-O(19)	72.62(12)	
O(5)#1-Ba(1)-O(4)#1	74.01(10)	O(7)-Ba(2)-O(5W)	73.15(19)	
O(1)-Ba(1)-O(4)#1	144.68(10)	O(6W)-Ba(2)-O(5W)	141.1(2)	
O(13)-Ba(1)-O(4)#1	70.06(10)	O(4W)-Ba(2)-O(5W)	78.1(2)	
O(2)-Ba(1)-O(2W)	121.33(8)	O(10)#2-Ba(2)-O(5W)	75.97(19)	
O(5)#1-Ba(1)-O(2W)	77.86(9)	O(8)-Ba(2)-O(5W)	131.51(17)	
O(1)-Ba(1)-O(2W)	80.63(9)	O(19)-Ba(2)-O(5W)	72.3(2)	
O(13)-Ba(1)-O(2W)	148.85(12)	O(7)-Ba(2)-O(3W)	90.81(14)	

	7	7	
O(6W)-Ba(2)-O(4W)	103.11(15)	O(1W)-Ba(1)-Ba(1)#1	42.32(10)
O(7)-Ba(2)-O(4W)	103.96(12)	O(7W)-Ba(1)-Ba(1)#1	38.3(2)
O(7)-Ba(2)-O(8)	72.39(10)	O(2W)-Ba(1)-Ba(1)#1	37.40(9)
O(4W)-Ba(2)-O(10)#2	72.21(11)	O(4)#1-Ba(1)-Ba(1)#1	106.93(7)
O(6W)-Ba(2)-O(10)#2	67.83(11)	O(13)-Ba(1)-Ba(1)#1	173.72(8)
O(7)-Ba(2)-O(10)#2	148.97(12)	O(1)-Ba(1)-Ba(1)#1	107.28(7)
Ba(1)#1	41.57(9)	O(5)#1-Ba(1)-Ba(1)#1	103.81(7)
O(1W)#1-Ba(1)-			
O(7W)-Ba(1)-O(1W)#1	50.63(17)	O(2)-Ba(1)-Ba(1)#1	102.90(7)
O(2W)-Ba(1)-O(1W)#1	56.78(11)	O(7W)-Ba(1)-O(1W)	51.08(17)
O(1W)#1	134.11(14)	O(2W)-Ba(1)-O(1W)	57.30(11)
O(4)#1-Ba(1)-			
O(13)-Ba(1)-O(1W)#1	136.81(11)	O(4)#1-Ba(1)-O(1W)	69.26(11)
O(1)-Ba(1)-O(1W)#1	79.36(14)	O(13)-Ba(1)-O(1W)	137.12(12)
O(1W)#1	134.39(12)	O(1)-Ba(1)-O(1W)	137.25(12)
O(5)#1-Ba(1)-			
O(2)-Ba(1)-O(1W)#1	66.41(11)	O(5)#1-Ba(1)-O(1W)	75.54(14)
O(2W)-Ba(1)-O(7W)	75.7(2)	O(2)-Ba(1)-O(1W)	130.77(15)
O(4)#1-Ba(1)-O(7W)	83.83(16)	O(5W)-Ba(2)-O(3W)	142.6(2)
O(13)-Ba(1)-O(7W)	135.4(2)	O(19)-Ba(2)-O(3W)	141.69(13)
O(1)-Ba(1)-O(7W)	129.80(12)	O(8)-Ba(2)-O(3W)	70.20(12)
O(5)#1-Ba(1)-O(7W)	126.55(13)	O(10)#2-Ba(2)-O(3W)	116.20(14)
O(2)-Ba(1)-O(7W)	79.95(15)	O(4W)-Ba(2)-O(3W)	73.35(14)
O(4)#1-Ba(1)-O(2W)	124.09(7)	O(6W)-Ba(2)-O(3W)	70.11(14)

Sr(1)-O(2)	2.577(3)	Sr(1)-O(1W)	2.598(3)
Sr(1)-O(4)#1	2.558(2)	Sr(1)-O(2W)	2.570(3)
Sr(1)-O(5)#1	2.541(2)	Sr(1)-O(3W)	2.627(3)
Sr(1)-O(7)	2.522(3)	Sr(1)-O(4W)	2.641(3)
O(7)-Sr(1)-O(5)#1	98.74(11)	O(2)-Sr(1)-O(1W)	67.59(8)
O(7)-Sr(1)-O(4)#1	77.35(9)	O(7)-Sr(1)-O(3W)	149.60(10)
O(5)#1-Sr(1)-O(4)#1	79.15(8)	O(5)#1-Sr(1)-O(3W)	82.08(9)
O(7)-Sr(1)-O(2W)	139.82(10)	O(4)#1-Sr(1)-O(3W)	72.95(9)
O(5)#1-Sr(1)-O(2W)	75.32(8)	O(2W)-Sr(1)-O(3W)	70.06(9)
O(4)#1-Sr(1)-O(2W)	137.27(8)	O(2)-Sr(1)-O(3W)	116.28(9)
O(7)-Sr(1)-O(2)	78.55(10)	O(1W)-Sr(1)-O(3W)	70.94(9)
O(5)#1-Sr(1)-O(2)	147.97(8)	O(7)-Sr(1)-O(4W)	68.17(13)
O(4)#1-Sr(1)-O(2)	129.87(8)	O(5)#1-Sr(1)-O(4W)	72.58(11)
O(2W)-Sr(1)-O(2)	86.30(8)	O(4)#1-Sr(1)-O(4W)	130.57(11)
O(7)-Sr(1)-O(1W)	93.36(12)	O(2W)-Sr(1)-O(4W)	72.24(12)
O(5)#1-Sr(1)-O(1W)	144.11(8)	O(2)-Sr(1)-O(4W)	76.96(10)
O(4)#1-Sr(1)-O(1W)	70.72(8)	O(1W)-Sr(1)-O(4W)	142.80(11)
O(2W)-Sr(1)-O(1W)	114.91(9)	O(3W)-Sr(1)-O(4W)	138.70(12)
	:	8	
Ca(1)-O(1)	2.447(5)	Ca(1)-O(3W)	2.428(5)
Ca(1)-O(2)	2.421(5)	Ca(1)-O(4W)	2.423(5)
Ca(2)-O(5)	2.454(4)	Ca(1)-O(5W)	2.574(6)
Ca(1)-O(8)#1	2.491(4)	Ca(2)-O(6W)	2.461(5)
Ca(2)-O(10)#1	2.565(5)	Ca(2)-O(7W)	2.405(5)
Ca(2)-O(11)#1	2.352(4)	Ca(2)-O(8W)	2.533(6)

Ca(1)-O(1W)	2.440(6)	Ca(2)-O(9W)	2.404(5)
Ca(1)-O(2W)	2.479(5)	Ca(2)-O(10W)	2.402(5)
O(2)-Ca(1)-O(4W)	76.67(17)	O(2)-Ca(1)-O(8)#1	140.90(16)
O(2)-Ca(1)-O(3W)	148.01(17)	O(4W)-Ca(1)-O(8)#1	79.13(17)
O(4W)-Ca(1)-O(3W)	107.86(18)	O(3W)-Ca(1)-O(8)#1	69.29(16)
O(2)-Ca(1)-O(1W)	103.67(19)	O(1W)-Ca(1)-O(8)#1	82.42(17)
O(4W)-Ca(1)-O(1W)	148.94(19)	O(1)-Ca(1)-O(8)#1	134.12(16)
O(3W)-Ca(1)-O(1W)	88.37(19)	O(2W)-Ca(1)-O(8)#1	73.49(18)
O(2)-Ca(1)-O(1)	82.73(16)	O(2)-Ca(1)-O(5W)	81.36(18)
O(4W)-Ca(1)-O(1)	138.66(17)	O(4W)-Ca(1)-O(5W)	70.66(18)
O(3W)-Ca(1)-O(1)	73.35(16)	O(3W)-Ca(1)-O(5W)	71.07(18)
O(1W)-Ca(1)-O(1)	70.71(17)	O(1W)-Ca(1)-O(5W)	140.40(19)
O(2)-Ca(1)-O(2W)	72.37(18)	O(1)-Ca(1)-O(5W)	71.08(17)
O(4W)-Ca(1)-O(2W)	79.90(19)	O(2W)-Ca(1)-O(5W)	144.29(18)
O(3W)-Ca(1)-O(2W)	139.39(18)	O(8)#1-Ca(1)-O(5W)	118.46(19)
O(1W)-Ca(1)-O(2W)	70.97(19)	O(11)#1-Ca(2)-O(10W)	76.07(16)
O(1)-Ca(1)-O(2W)	127.00(19)	O(11)#1-Ca(2)-O(9W)	143.59(17)
O(9W)-Ca(2)-O(6W)	139.53(19)	O(10W)-Ca(2)-O(9W)	114.5(2)
O(7W)-Ca(2)-O(6W)	70.76(16)	O(11)#1-Ca(2)-O(7W)	100.60(17)
O(5)-Ca(2)-O(6W)	74.79(17)	O(10W)-Ca(2)-O(7W)	144.87(17)
O(11)#1-Ca(2)-O(8W)	81.19(18)	O(9W)-Ca(2)-O(7W)	89.2(2)
O(10W)-Ca(2)-O(8W)	71.89(17)	O(11)#1-Ca(2)-O(5)	144.55(17)
O(9W)-Ca(2)-O(8W)	70.6(2)	O(10W)-Ca(2)-O(5)	76.99(15)
O(7W)-Ca(2)-O(8W)	142.93(17)	O(9W)-Ca(2)-O(5)	69.77(16)
O(5)-Ca(2)-O(8W)	111.52(18)	O(7W)-Ca(2)-O(5)	88.54(17)

O(6W)-Ca(2)-O(8W)	143.07(18)	O(11)#1-Ca(2)-O(6W)	76.13(18)
O(11)#1-Ca(2)-			
O(10)#1	81.89(16)	O(10W)-Ca(2)-O(6W)	74.56(17)
O(10W)-Ca(2)-			
O(10)#1	139.29(16)	O(5)-Ca(2)-O(10)#1	133.22(15)
O(9W)-Ca(2)-O(10)#1	67.68(17)	O(6W)-Ca(2)-O(10)#1	132.24(16)
O(7W)-Ca(2)-O(10)#1	72.43(16)	O(8W)-Ca(2)-O(10)#1	71.20(16)
	ç)	
Sr(1)-O(1)	2.694(3)	Sr(1)-O(2W)	2.609(4)
Sr(1)-O(2)	2.542(3)	Sr(1)-O(3W)	2.723(4)
Sr(1)-O(13)	2.584(3)	Sr(1)-O(4W)	2.613(5)
Sr(1)-O(1W)	2.573(4)	Sr(1)-O(5W)	2.598(4)
O(2)-Sr(1)-O(1W)	82.74(14)	O(2)-Sr(1)-O(1)	80.85(9)
O(2)-Sr(1)-O(13)	75.69(11)	O(1W)-Sr(1)-O(1)	74.26(13)
O(1W)-Sr(1)-O(13)	132.89(15)	O(13)-Sr(1)-O(1)	139.79(10)
O(2)-Sr(1)-O(5W)	147.52(11)	O(5W)-Sr(1)-O(1)	68.32(11)
O(1W)-Sr(1)-O(5W)	79.38(16)	O(2W)-Sr(1)-O(1)	67.33(11)
O(13)-Sr(1)-O(5W)	135.39(13)	O(4W)-Sr(1)-O(1)	144.85(12)
O(2)-Sr(1)-O(2W)	88.39(12)	O(2)-Sr(1)-O(3W)	143.48(12)
O(1W)-Sr(1)-O(2W)	141.49(14)	O(1W)-Sr(1)-O(3W)	128.33(16)
O(13)-Sr(1)-O(2W)	79.70(11)	O(13)-Sr(1)-O(3W)	68.79(14)
O(5W)-Sr(1)-O(2W)	88.97(13)	O(5W)-Sr(1)-O(3W)	66.64(13)
O(2)-Sr(1)-O(4W)	106.75(15)	O(2W)-Sr(1)-O(3W)	77.40(15)
O(1W)-Sr(1)-O(4W)	72.84(15)	O(4W)-Sr(1)-O(3W)	71.81(17)
O(13)-Sr(1)-O(4W)	74.14(14)	O(1)-Sr(1)-O(3W)	122.12(13)

^a Symmetry transformations used to generate equivalent atoms: #1 x-1, y, z; #2 -x+1, -y+1, -z
for 1; #1 x+1, y, z for 2; #1 -x+2, -y+1, -z+1; #2 x+1, y, z for 3; #1 x, y+1, z; #2 -x, -y, -z+1 for
4; #1 -x+1, -y+1, -z+1; #2 x, y+1, z for 5; #1 -x+1, y, -z+3/2; #2 -x+3/2, -y+3/2, -z+2 for 6;
#1 x+1, y, z for 7; #1 x, y, z-1; #2 x, y, z+1 for 8.

adsorbent	$K_{SV}(\mathrm{M}^{-1})$	Reference
Tb-DSOA	3.543×10^{3}	1
Eu-MOF/EDTA-NiAl-CLDH–M	8.22×10^{3}	2
BUT-14	2.17×10^{3}	3
BUT-15	1.66 ×10 ³	
${[Eu_3(pdba)_4(H_2O)_4] \cdot 5H_2O}_n$	5.8×10^{3}	4
$[Zn_2(cptpy)(btc)(H_2O)]_n$	1.038×10^{3}	5
534-MOF-Tb	5.51×10^{3}	6
$[Cd_3(dpa)(DMF)_2 (H_2O)_3] \cdot DMF$	5.30 × 10 ³	7
$[NaCd_2(L)(BDC)_{2.5}] \cdot 9H_2O$	4.48×10^{3}	
$[Cd_2(L)(2,6-NDC)_2] \cdot DMF \cdot 5H_2O$	4.36×10^{3}	8
$[Cd_2(L)(BPDC)_2] \cdot DMF \cdot 9H_2O$	2.52×10^{3}	
2	4.32×10^{3}	This study
7	4.16×10^{3}	This study

Table S2. Comparison of the quenching constants (K_{SV}) for the detection of Fe³⁺ of some reported MOFs-based materials.

		2	7
	1	1001.54812	945.2371
	2	1001.52606	945.3943
Fluorescence intensity without analytes	3	1001.67462	945.1528
	4	1001.59083	945.1965
	5	1001.50237	945.2296
Standard deviation (σ)		0.06058	0.08175
$K_{SV}(\mathrm{M}^{-1})$		4.32×10 ³	4.16×10 ³
Detection limit $(3\sigma/K_{SV}, M)$		1.40×10 ⁻⁵	1.96×10 ⁻⁵

Table S3. The calculation of the detection limits of 2 and 7 for Fe^{3+} .

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