Electronic Supplementary Material (ESI) for CrystEngComm.


# Supplementary information

# Gas Adsorption, Magnetic Properties and Fluorescent Sensing of Four Coordination Polymers Based on 1,3,5–Tris(4-carbonylphenyloxy)benzene and Bis(imidazole) Linkers

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**Table S1.** Crystallographic data for **1**, **2**, **3** and **4**.

| Complex | **1** | **2** | **3** | **4** |
|---|---|---|---|---|
| Empirical formula | $C_{90}H_{58}Co_3N_8O_{18}$ | $C_{188}H_{132}N_6O_{42}Cd_6$ | $C_{75}H_{51}Co_3N_6O_{18}$ | $C_{76}H_{60}N_4O_{22}Zn_3$ |
| Formula weight | 1716.23 | 3961.55 | 1501.01 | 1577.39 |
| Crystal system | Triclinic | monoclinic | Triclinic | Triclinic |
| Space group | *P-1* | C2/c | *P*-1 | *P-1* |
| *a* [Å] | 15.849(8) | 65.582(4) | 10.5993(6) | 10.3103(6) |
| *b* [Å] | 16.159(1) | 30.419(2) | 12.1538(8) | 12.3541(7) |
| *c* [Å] | 23.670(1) | 16.936(7) | 14.4103(8) | 14.4917(9) |
| *α* [°] | 97.696(2) | 90 | 86.666(3) | 86.150(2) |
| *β* [°] | 92.686(2) | 90.001(0) | 69.331(2) | 70.328(2) |
| *γ* [°] | 112.973(2) | 90 | 87.296(3) | 86.391(2) |
| *V* [Å$^3$] | 5498(5) | 33788(4) | 1733.23(18) | 1732.62(18) |
| *Z* | 2 | 8 | 1 | 1 |
| *D*c / (g·cm$^{-3}$) | 1.037 | 1.558 | 1.438 | 1.512 |
| *F*(000) | 11758.0 | 15967.0 | 768.0 | 810.0 |
| $\mu$(Mo *K*α) / mm$^{-1}$ | 0.504 | 0.829 | 0.71073 | 0.71073 |
| Reflections collected | 128968 | 280982 | 28127 | 35798 |
| $\theta$ range for data collection / (°) | 2.262-25.449 | 2.214-25.027 | 2.08-26.179 | 3.309- 27.521 |
| Independent reflections ($R_{int}$) | 20250 (0.0960) | 29843(0.1198) | 6879(0.0859) | 7977(0.0879) |
| Data / restraints / parameters | 20250/0/1072 | 29843/2568/2437 | 6879/132/493 | 7977/73/475 |
| Gof | 1.024 | 1.077 | 1.023 | 1.034 |
| $R_1$, $wR_2$ [$I$>2$\sigma(I)$]$^{ab}$ | 0.0715, 0.1148 | 0.0870, 0.1907 | 0.0730,0.1959 | 0.0511 0.1346 |
| $R_1$, $wR_2$ (all data)$^a$ | 0.1265, 0.1673 | 0.1337, 0.2232 | 0.1290,0.2361 | 0.0662, 0.1452 |
| Largest diff. Peak and hole[e·Å$^{-3}$] | 0.38 and -0.37 | 2.36 and -2.75 | 1.67 and-0.75 | 0.95 and-0.55 |
| CCDC number | 1576190 | 1576192 | 1848568 | 1848570 |

$^aR_1=\Sigma||F_o|-|F_c|/\Sigma||F_o|$. $^bwR_2 = \{[\Sigma w(F_o2-F_c^2)^2/\Sigma w(F_o^2)^2]\}^{1/2}$.

**Table. S2** Selected bond lengths/Å and bond angles/°for complex (**1**), (**2**), (**3**) and (**4**)

| Complex 1 | | | | | |
|---|---|---|---|---|---|
| Co1–O1$^{i}$ | 2.124(3) | Co1–O5$^{i}$ | 2.082(3) | Co1–O8$^{ii}$ | 2.070(3) |
| Co1–O10 | 2.063(3) | Co1–O14$^{iii}$ | 2.122(3) | Co1–O17$^{ii}$ | 2.080(3) |
| Co2–O1$^{iv}$ | 2.147(3) | Co2–O2$^{iv}$ | 2.209(3) | Co2–O4$^{v}$ | 2.058(3) |
| Co2–O7 | 2.054(3) | Co2–N4 | 2.136(4) | Co2–N8$^{vi}$ | 2.065(3) |
| Co3–O11$^{v}$ | 2.061(3) | Co3–O14$^{vii}$ | 2.171(3) | Co3–O15$^{vii}$ | 2.149(3) |

| | | | | | |
|---|---|---|---|---|---|
| Co3–O18 | 2.070(3) | Co3–N1$^{v}$ | 2.119(4) | Co3–N5 | 2.054(3) |
| O5–Co1–O1$^{i}$ | 92.10(1) | O5–Co1–O14$^{ii}$ | 84.55(1) | O8$^{iii}$–Co1–O11$^{i}$ | 89.31(1) |
| O8$^{iii}$–Co1–O5 | 94.56(1) | O8$^{iii}$–Co1–O14$^{ii}$ | 89.75(1) | O8$^{iii}$–Co1–O17$^{iii}$ | 85.07(1) |
| O10–Co1–O1$^{i}$ | 90.79(1) | O10–Co1–O5 | 94.56(1) | O10–Co1–O8$^{iii}$ | 179.47(1) |
| O10–Co1–O14$^{ii}$ | 90.19(1) | O10–Co1–O17$^{iii}$ | 94.31(1) | O14$^{ii}$–Co1–O1$^{i}$ | 90.79(1) |
| O17$^{iii}$–Co1–O1$^{i}$ | 85.40(1) | O17$^{iii}$–Co1–O5 | 177.49(1) | O17$^{iii}$–Co1–O14$^{ii}$ | 97.95(1) |
| O17$^{iii}$–Co1–O14$^{ii}$ | 97.95(1) | O1$^{4}$–Co2–O2$^{iv}$ | 59.95(1) | O4$^{v}$–Co2–O1$^{iv}$ | 89.17(1) |
| O4$^{v}$–Co2–O2$^{iv}$ | 86.74(1) | O4$^{v}$–Co2–N4 | 173.37(1) | O4$^{v}$–Co2–N8$^{vi}$ | 93.97(1) |
| O7–Co2–O1$^{iv}$ | 108.19(1) | O7–Co2–O4$^{v}$ | 92.44(1) | O7–Co2–N4 | 85.94(1) |
| O17$^{v}$–Co2–N8$^{vi}$ | 97.09(1) | N8$^{vi}$–Co2–O1$^{iv}$ | 85.14(1) | N8$^{vi}$–Co2–O2$^{iv}$ | 94.81(1) |
| O12$^{i}$–Co3–N4 | 92.61(1) | O11$^{v}$–Co3–O14$^{vii}$ | 107.27(1) | O11$^{v}$–Co3–O18 | 90.73(1) |
| O11$^{v}$–Co3–O18 | 90.73(1) | O11$^{v}$–Co3–N1$^{v}$ | 86.99(1) | O15$^{vii}$–Co3–O14$^{vii}$ | 61.09(1) |
| O18–Co3–O14$^{vii}$ | 87.35(1) | O18–Co3–O15$^{vii}$ | 92.13(1) | O18–Co3–N1$^{v}$ | 171.99(1) |
| N1$^{v}$–Co3–O14$^{vii}$ | 86.00(1) | N1$^{v}$–Co3–O14$^{vii}$ | 92.13(1) | N5–Co3–O11$^{v}$ | 95.36(1) |
| N5–Co3–O14$^{vii}$ | 156.78(1) | N5–Co3–O15$^{vii}$ | 96.20(1) | N5–Co3–O18 | 87.26(1) |
| N5–Co3–N1$^{v}$ | 100.60(1) | | | | |

Symmetry codes:$^{i}$1+x，1+y，+z; $^{ii}$+x，+y，1+z; $^{iii}$1+x，1+y，1+z; $^{iv}$1+x，+y，1+z;$^{v}$+x，1+y，+z; $^{vi}$+x,-1+y,1+z; $^{vii}$1+x，

**Complex 2**

| | | | | | |
|---|---|---|---|---|---|
| Cd1–O17 | 2.365(6) | Cd1–O18 | 2.483(6) | Cd1–O21 | 2.258(7) |
| Cd1–O19 | 2.361(6) | Cd1–O20 | 2.454(7) | Cd1–O2$^{viii}$ | 2.374(7) |
| Cd2–O22 | 2.238(7) | Cd2–O38$^{xi}$ | 2.323(7) | Cd2–O2W | 2.273(9) |
| Cd2–O37$^{xi}$ | 2.425(7) | Cd2–O23 | 2.421(9) | Cd3–N10 | 2.270(9) |
| Cd3–O19$^{viii}$ | 2.420(7) | Cd3–O1 | 2.466(7) | Cd3–O2 | 2.478(6) |
| Cd3–O36$^{ix}$ | 2.429(7) | Cd3–O35$^{ix}$ | 2.719(8) | Cd4–O13 | 2.407(6) |
| Cd4–O14 | 2.260(6) | Cd4–O15 | 2.475(6) | Cd4–O16 | 2.260(7) |
| Cd5–O3$^{vi}$ | 2.455(6) | Cd5–O6$^{vi}$ | 2.569(6) | Cd5–O5$^{vi}$ | 2.307(6) |
| Cd5–O29$^{vii}$ | 2.610(6) | Cd5–O28$^{vii}$ | 2.349(6) | Cd6–O31$^{ii}$ | 2.444(6) |
| Cd6–O3$^{iii}$ | 2.389(6) | Cd6–O30$^{ii}$ | 2.331(6) | Cd6–O4$^{iii}$ | 2.398(6) |
| Cd6–O4$^{iii}$ | 2.398(6) | Cd6–O29$^{iv}$ | 2.363(6) | Cd6–O15$^{v}$ | 2.272(6) |
| Cd1–N13 | 2.297(8) | Cd2–N7$^{xii}$ | 2.283(1) | Cd3–N11$^{x}$ | 2.275(8) |
| Cd5–N5 | 2.269(7) | Cd5–N4 | 2.308(8) | Cd6–N1 | 2.323(8) |
| O17–Cd1– O18 | 53.8(2) | O17–Cd1–O2$^{viii}$ | 91.6(2) | O1–Cd1–O20 | 135.0(2) |
| O22–Cd2–O38$^{xi}$ | 132.2(3) | O22–Cd2–O37$^{xi}$ | 170.8(3) | O22–Cd2–O23 | 85.3(4) |
| O22–Cd2–N7$^{xii}$ | 87.3(4) | O38$^{xi}$–Cd2–O37$^{xi}$ | 55.5(2) | O22–Cd2–O2W | 97.5(3) |
| O38$^{xi}$–Cd2–O23 | 142.4(3) | O23–Cd2–O37$^{xi}$ | 87.0(3) | O2W–Cd2–O38$^{xi}$ | 96.3(3) |
| O2W–Cd2–O37$^{xi}$ | 85.8(3) | O2W–Cd2–O23 | 77.6(3) | O2W–Cd2–N7$^{xii}$ | 163.9(4) |
| N7$^{xii}$–Cd2–O38$^{xi}$ | 91.8(4) | N7$^{xii}$–Cd2–O37$^{xi}$ | 87.3(3) | N7$^{xii}$–Cd2–O23 | 87.4(4) |
| O2–Cd3–Cd1$^{viii}$ | 37.90(1) | O1–Cd3–O2 | 52.9(2) | O19$^{viii}$–Cd3–O2 | 74.7(2) |
| O19$^{viii}$–Cd3–O1 | 127.2(2) | O19$^{viii}$–Cd3–O36$^{ix}$ | 140.4(2) | O35 $^{ix}$–Cd3–O2 | 160.0(2) |
| O35$^{ix}$–Cd3–O1 | 146.8(2) | O35$^{ix}$–Cd3–O19$^{viii}$ | 85.9(2) | O35$^{ix}$–Cd3–O36$^{ix}$ | 54.7(2) |
| O35$^{ix}$–Cd3–C62 | 54.7(2) | O36$^{ix}$–Cd3–O2 | 144.9(2) | O36$^{ix}$–Cd3–O1 | 92.1(2) |
| N11$^{x}$–Cd3–O2 | 89.7(3) | N11$^{x}$–Cd3–O1 | 85.0(3) | N11$^{x}$– Cd3–O19$^{viii}$ | 90.3(3) |
| N11$^{x}$–Cd3–O35$^{ix}$ | 95.1(3) | N11$^{x}$–Cd3–O36$^{ix}$ | 89.8(3) | N10–Cd3–O2 | 87.2(3) |
| N10–Cd3–O1 | 92.4(3) | N10–Cd3–O19$^{viii}$ | 90.3(3) | N10–Cd3–O35$^{ix}$ | 88.0(3) |
| N10–Cd3–O36$^{ix}$ | 92.3(3) | O13–Cd4–O15 | 101.7(2) | O14–Cd4–O13 | 56.1(2) |
| O14– Cd4– O16 | 128.0(3) | O14–Cd4–N16 | 102.6(3) | O16–Cd4–O13 | 165.9(2) |

| | | | | | |
|---|---|---|---|---|---|
| O16– Cd4– O15 | 55.0(2) | O16–Cd4–N16 | 83.8(3) | O1W–Cd4–O13 | 90.0(3) |
| O1W–Cd4–O14 | 132.0(3) | O1W–Cd4–O15 | 81.8(3) | O1W– Cd4–O16 | 93.5(3) |
| O1W–Cd4–N16 | 105.1(3) | O3$^{vi}$–Cd5–O6$^{vi}$ | 139.0(7) | O3$^{vi}$–Cd5–O29$^{vii}$ | 73.5(8) |
| O6$^{vi}$–Cd5–O29$^{vii}$ | 146.1(2) | O5$^{vi}$–Cd5–O3$^{vi}$ | 86.0(2) | O5$^{vi}$–Cd5–O6$^{vi}$ | 53.3(2) |
| O5$^{vi}$–Cd5–O29$^{vii}$ | 158.8(2) | O5$^{vi}$– Cd5–O28$^{vii}$ | 149.1(2) | O5$^{vi}$–Cd5–N4 | 91.9(3) |
| O28$^{vii}$–Cd5–O3$^{vi}$ | 124.2(2) | O28$^{vii}$–Cd5–O6$^{vi}$ | 88.8(2) | O28$^{vii}$–Cd5–O29$^{vii}$ | 52.0(6) |
| N5–Cd5–O3$^{vi}$ | 84.1(2) | N5–Cd5–O6$^{vi}$ | 88.8(2) | N4–Cd5–O3$^{vi}$ | 89.6(2) |
| N5–Cd5–O5$^{vi}$ | 86.5(3) | N5–Cd5–O29$^{vii}$ | 85.9(2) | N5–Cd5–O29$^{vii}$ | 85.9(2) |
| N5–Cd5–O28$^{vii}$ | 101.6(2) | N4–Cd5–O6$^{vi}$ | 95.1(3) | O30$^{i}$–Cd6–O31$^{i}$ | 54.6(2) |
| O30$^{i}$–Cd6–O3$^{iii}$ | 165.0(2) | O30$^{i}$–Cd6–O29$^{iv}$ | 88.2(2) | O30$^{i}$–Cd6–O4$^{iii}$ | 54.8(2) |
| O3$^{iii}$–Cd6–O4$^{iii}$ | 54.8(2) | O29$^{iii}$–Cd6–O3$^{iii}$ | 79.4(2) | O3$^{iii}$–Cd6–O31$^{i}$ | 138.0(2) |
| O29$^{iii}$–Cd6–O31$^{i}$ | 142.5(2) | O15$^{v}$–Cd6–O30$^{i}$ | 98.0(2) | O15$^{v}$–Cd6–O31$^{i}$ | 89.7(2) |
| O15$^{v}$–Cd6–O3$^{iii}$ | 90.8(2) | O15$^{v}$–Cd6–O29$^{iv}$ | 91.9(2) | O15$^{v}$–Cd6–O4$^{iii}$ | 91.6(2) |
| O15$^{v}$–Cd6–N1 | 175.0(3) | O4$^{iii}$–Cd6–O30$^{i}$ | 83.2(2) | N1–Cd6–O31$^{i}$ | 94.6(3) |
| N1–Cd6–O3$^{iii}$ | 87.6(2) | N1–Cd6–O29$^{iv}$ | 83.2(2) | N1–Cd6–O4$^{iii}$ | 91.3(3) |

Symmetry codes: $^{i}$1-*x*，-*y*，-*z*$^{ii}$，-1+*x*，-*y*，+*z*$^{iii}$;1+*x*，1+*y*，+*z*

**Complex 3**

| | | | | | |
|---|---|---|---|---|---|
| Co1-O1 | 2.056(4) | Co1-O8$^{v}$ | 2.052(4) | Co2-O5$^{iii}$ | 2.191(4) |
| Co1-O1$^{i}$ | 2.056(4) | Co2-O2 | 2.064(4) | Co2-O6$^{iii}$ | 2.124(4) |
| Co1-O5$^{ii}$ | 2.107(4) | Co1-O8$^{iv}$ | 2.052(4) | Co2-O9$^{iv}$ | 1.969(5) |
| Co1-O5$^{iii}$ | 2.107(4) | | | | |
| O1-Co1-O1$^{i}$ | 180.0 | O8$^{iv}$-Co1-O5$^{iii}$ | 89.53(17) | N1-Co2-O5$^{iii}$ | 158.34(17) |
| O1-Co1-O5$^{ii}$ | 87.85(16) | O8$^{v}$-Co1-O5$^{iii}$ | 90.47(17) | N1-Co2-O6$^{iii}$ | 98.26(17) |
| O1$^{i}$-Co1-O5$^{ii}$ | 92.15(15) | O8$^{v}$-Co1-O8$^{iv}$ | 180.0 | N1-Co2-N3 | 94.7(3) |
| O1$^{i}$-Co1-O5$^{iii}$ | 87.85(16) | O2-Co2-O5$^{iii}$ | 94.92(16) | O8$^{v}$-Co1-O5$^{ii}$ | 89.53(17) |
| O1-Co1-O5$^{iii}$ | 92.15(16) | O2-Co2-O6$^{iii}$ | 101.59(19) | O9$^{v}$-Co2-N3 | 73.1(4) |
| O5$^{iii}$-Co1-O5$^{ii}$ | 180.00(12) | O2-Co2-N3 | 172.8(4) | Co1$^{vi}$-O5-Co2$^{v}$ | 110.27(17) |
| O8$^{iv}$-Co1-O1 | 86.91(18) | O5$^{iii}$-Co2-N3 | 82.6(3) | O9$^{v}$-Co2-O5$^{iii}$ | 98.20(17) |
| O8$^{v}$-Co1-O1$^{i}$ | 86.91(18) | O6$^{iii}$-Co2-O5$^{iii}$ | 60.10(15) | O9$^{v}$-Co2-O6$^{iii}$ | 150.0(2) |
| O8$^{iv}$-Co1-O1$^{i}$ | 93.09(18) | O6$^{iii}$-Co2-N3 | 83.1(3) | O9$^{v}$-Co2-N1 | 101.55(18) |
| O8$^{v}$-Co1-O1 | 93.09(18) | O9$^{v}$-Co2-O2 | 100.7(2) | N1-Co2-O2 | 90.08(16) |
| O8$^{iv}$-Co1-O5$^{ii}$ | 90.47(17) | | | | |

Symmetry codes:$^{i}$-X,-Y,2-Z; $^{ii}$1-X,1-Y,1-Z; $^{iii}$-1+X,-1+Y,1+Z;$^{iv}$-1+X,+Y,1+Z; $^{v}$1-X,-Y,1-Z; $^{vi}$1+X,1+Y,-1+Z; $^{vii}$1+X,+Y,-1+Z; $^{viii}$-1-X,-Y,1-Z;$^{ix}$-1-X,-1-Y,2-Z

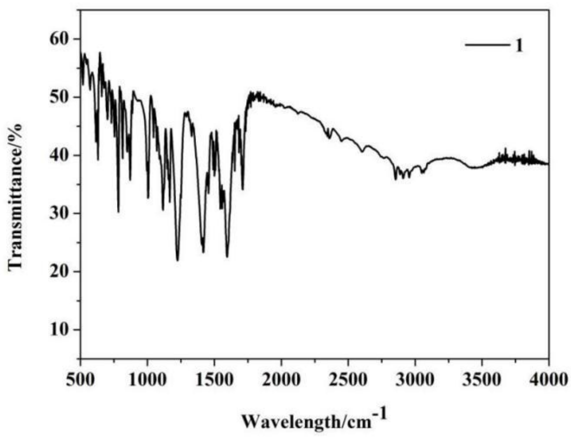
**Complex 4**

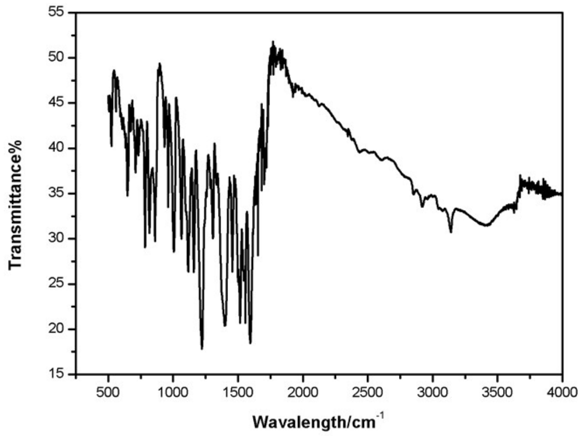
| | | | | | |
|---|---|---|---|---|---|
| Zn1-O1$^{i}$ | 2.236(4) | Zn1-O9$^{v}$ | 2.283(4) | Zn2-O7$^{i}$ | 2.415(4) |
| Zn1-O1 | 2.236(4) | Zn1-O9$^{v}$ | 2.283(4) | Zn2-O10 | 2.186(4) |
| Zn1-O6$^{ii}$ | 2.292(3) | Zn2-O2 | 2.211(4) | Zn2-N1 | 2.357(6) |
| Zn1-O6$^{iii}$ | 2.292(3) | Zn2-O6$^{ii}$ | 2.339(3) | Zn2-N2 | 2.340(5) |
| O1$^{i}$-Zn1-O1 | 180.0 | O9$^{v}$-Zn1-O6 $^{ii}$ | 84.90(12) | O6 $^{iii}$-Zn2-N1 | 92.25(18) |
| O1-Zn1-O6 $^{ii}$ | 90.37(13) | O9 $^{iv}$-Zn1-O6 $^{iii}$ | 84.90(12) | O6 $^{iii}$-Zn2-N2 | 136.90(13) |
| O1$^{i}$-Zn1-O6 $^{iii}$ | 90.37(13) | O9 $^{iv}$-Zn1-O9$^{v}$ | 180.0 | N2-Zn2-O7 $^{iii}$ | 87.09(14) |
| O1$^{i}$-Zn1-O6 $^{ii}$ | 89.63(13) | O2-Zn2-O6 $^{iii}$ | 101.36(15) | N1-Zn2-O7 $^{iii}$ | 94.99(19) |
| O1-Zn1-O6 $^{iii}$ | 89.63(13) | O2-Zn2-O7 $^{iii}$ | 155.63(15) | O10$^{v}$-Zn2-O2 | 92.08(16) |
| O1$^{i}$-Zn1-O9 $^{iv}$ | 90.68(14) | O2-Zn2-N1 | 88.0(2) | O10$^{v}$-Zn2-O6 $^{iii}$ | 111.11(15) |
| O1-Zn1-O9 $^{iv}$ | 89.32(14) | O2-Zn2-N2 | 116.52(16) | O10$^{v}$-Zn2-O7 $^{iii}$ | 94.70(16) |
| O1-Zn1-O9$^{v}$ | 90.68(14) | O9 $^{iv}$-Zn1-O6 $^{ii}$ | 95.10(12) | O10$^{v}$-Zn2-N1 | 156.1(2) |
| O1$^{i}$-Zn1-O9$^{v}$ | 89.32(14) | O6 $^{iii}$-Zn2-O7 $^{iii}$ | 54.42(12) | O10$^{v}$-Zn2-N2 | 88.30(18) |
| O6 $^{iii}$-Zn1-O6 $^{ii}$ | 180.0 | N2-Zn2-N1 | 70.5(2) | O9$^{v}$-Zn1-O6 $^{iii}$ | 95.10(12) |

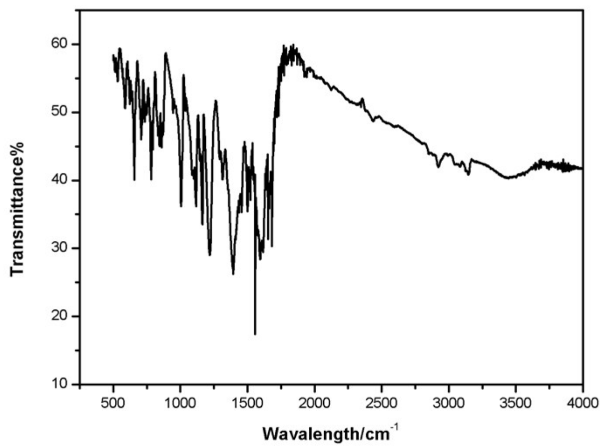
Symmetry codes: [i]-1-X,2-Y,1-Z; [ii]-1+X,+Y,1+Z; [iii]-X,1-Y,1-Z;[iv]-2-X,1-Y,1-Z; [v]-X,2-Y,-Z; [vi]-1+X,1+Y,+Z;[vii]1+X,+Y,-1+Z; [Viii]1+X,-1+Y,+Z

**Table S3.** Related parameters in the sensing of $Fe^{3+}$/$Cr^{3+}$ ions in **2** and **4**.

| | Quenching rate | Exponential equation | $K_{sv}$ ($M^{-1}$) | The detection limit |
|---|---|---|---|---|
| **1** for $Fe^{3+}$ | 97.85% (0.200 mM) | $I_0/I=15.05e^{9794[Fe3+]}-4.02$ | $7.8\times10^4$ | $1.02\times10^{-3}$ |
| **1** for $Cr^{3+}$ | 98.25% (0.200 mM) | $I_0/I=16.93e^{7304[Cr3+]}-16.64$ | $8.3\times10^4$ | $9.63\times10^{-3}$ |
| **2** for $Fe^{3+}$ | 96.08% (0.300 mM) | $I_0/I=15.63e^{3183[Fe3+]}-14.86$ | $7.8\times10^4$ | $1.16\times10^{-3}$ |
| **2** for $Cr^{3+}$ | 96.87% (0.300 mM) | $I_0/I=1.04+102.56$ [Cr3+] | $1.0\times10^5$ | $8.87\times10^{-4}$ |





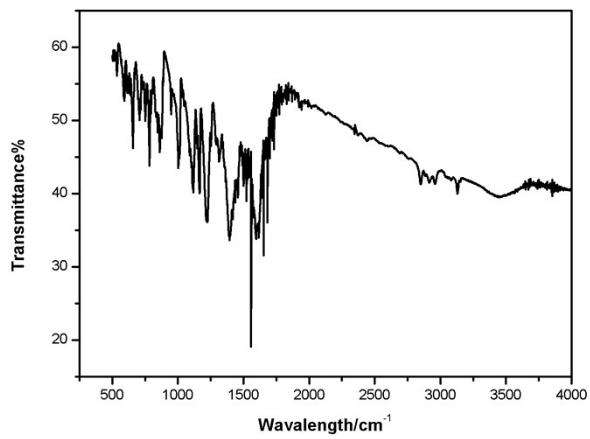




**Fig. S1.** The IR spectra of the complexes **1-4**.

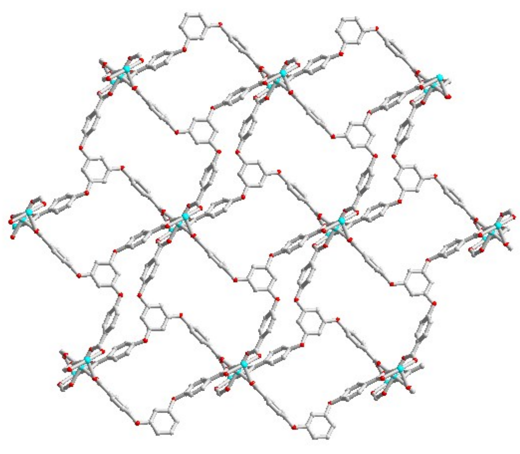


**Fig. S2.** The 2D $[Co(Htcpb)]_n$ network based on $Htcpb^{3-}$ and $Co^{II}$ ions.

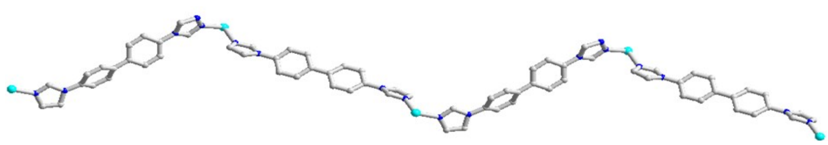
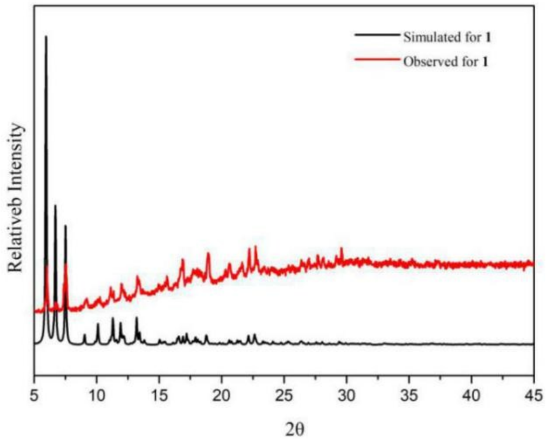
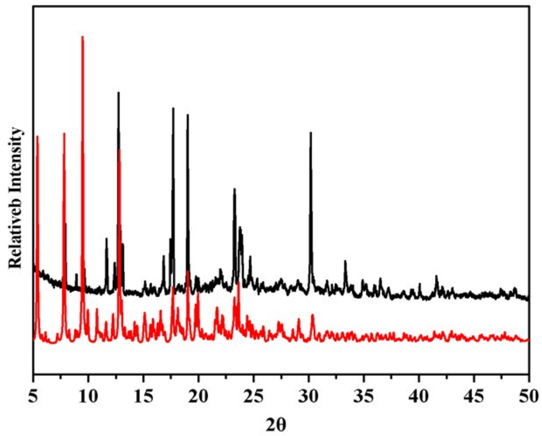
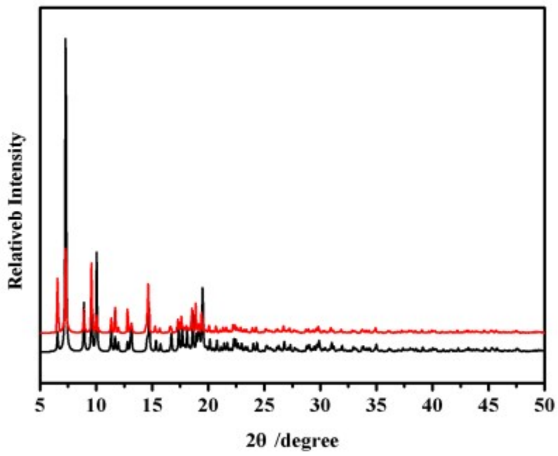


**Fig. S3.** 1D $[Co(4bib)]_n$ wavy linear chain formed by bib and $Co^{II}$ ions.


Simulated for 1
Observed for 1
Relativeb Intensity
5
10
15
20
25
30
35
40
45
2θ


Relativeb Intensity
5
10
15
20
25
30
35
40
45
50
2θ


Relativeb Intensity
5
10
15
20
25
30
35
40
45
50
2θ /degree

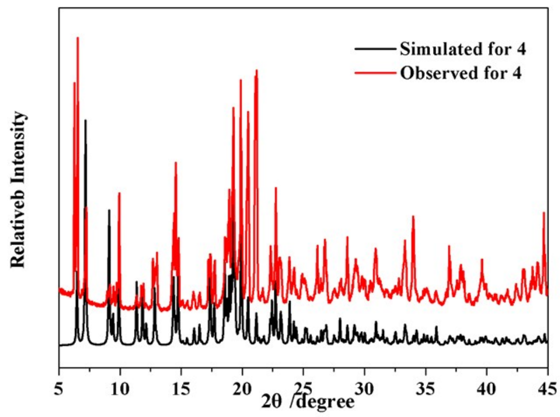



**Fig. S4.** PXRD patterns of the series complexes. Black: Simulated from the X–ray single–crystal data; Red: observed for the as–synthesized solids.

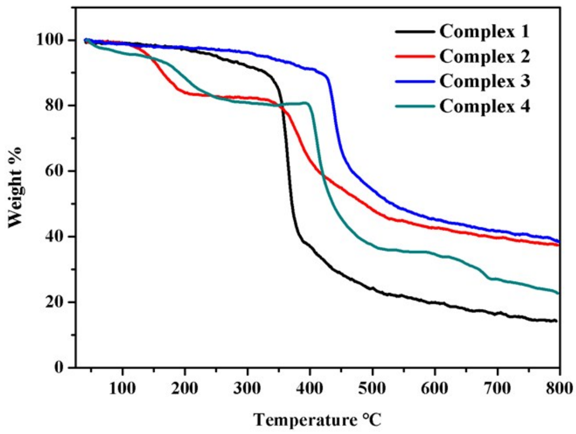



**Fig. S5.** The TG curve of complex **3**.

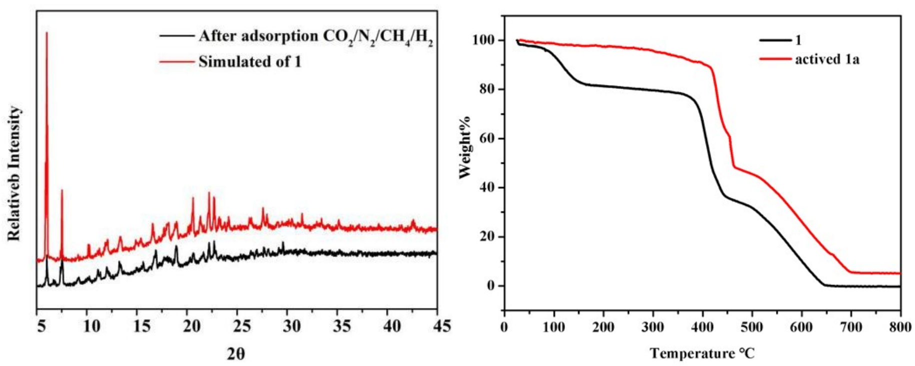
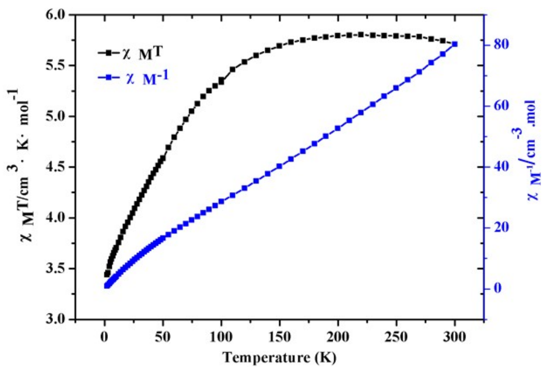
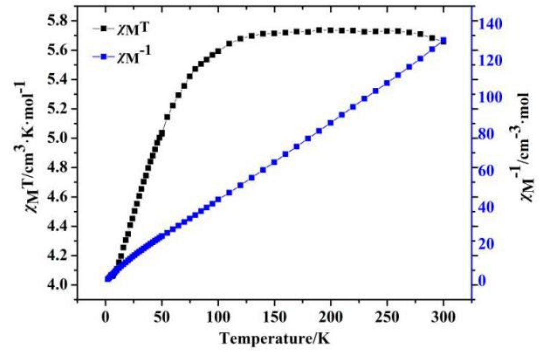



**Fig. S6**. The TG and PXRD of **1** under varied conditions




(a)




(b)

**Fig. S7.** Temperature dependence of $\chi_M$T and $\chi_M^{-1}$ for **2** (a) and **4** (b) at 1000

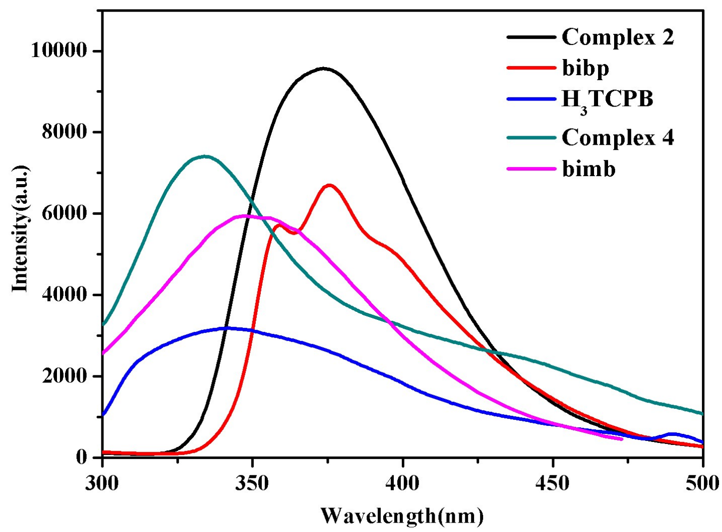



**Fig. S8.** Solid-state fluorescent emissions for $H_3$TCPB, bibp, bimb and **2** and **4** at room temperature.

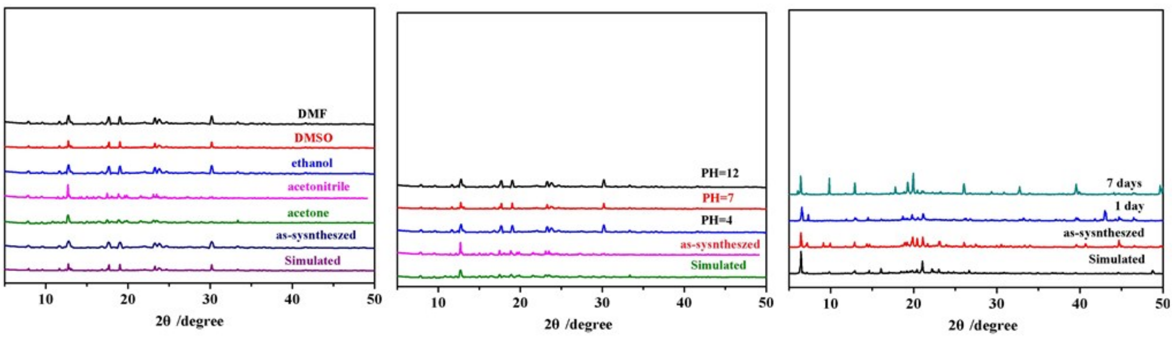



**Fig. S9.** PXRD patterns of **2** for the simulated, as-synthesized and after treated by various conditions.

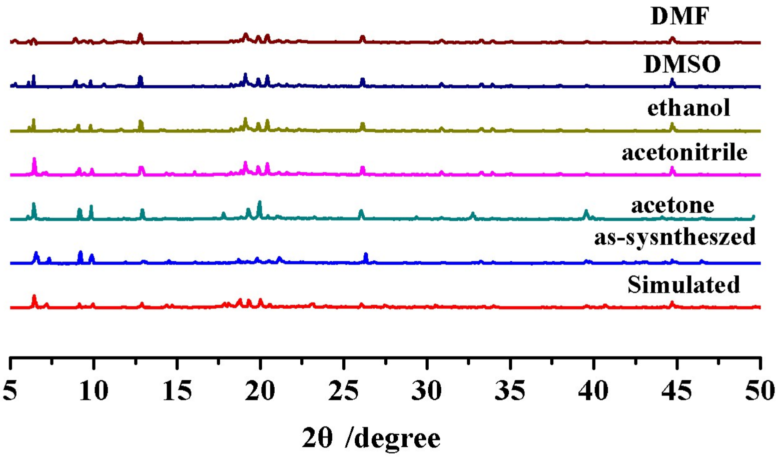



**Fig. S10.** PXRD patterns of **4** immersed in different solvents at room temperature.

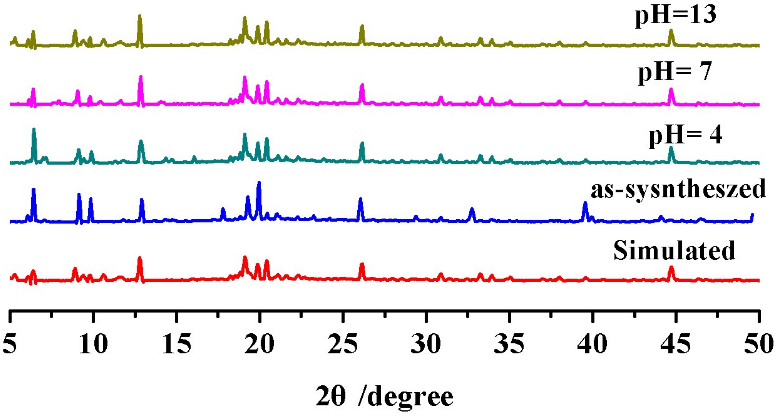



**Fig. S11.** PXRD patterns of **4** immersed in different pH solutions.

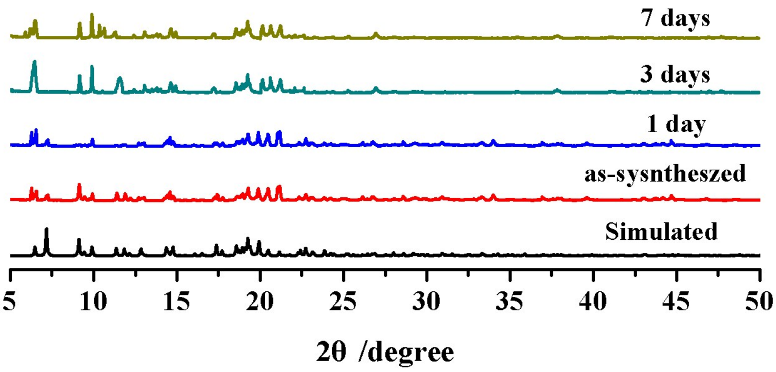



**Fig. S12.** The PXRD patterns of **4** for the simulated, as-synthesized and after water treated samples.

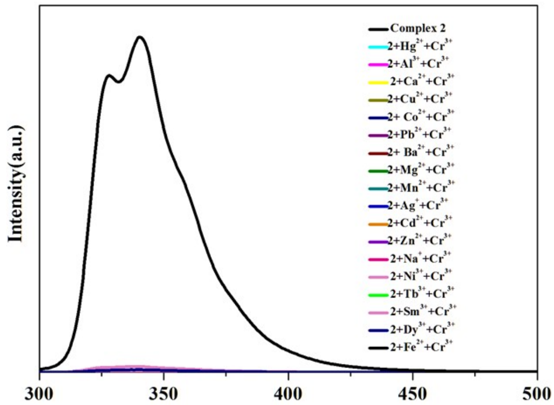



**Fig. S13.** Effect on the emission spectra of **2** dispersed in $H_2O$ upon incremental addition of $Cr^{3+}$ cations(1 mM) and the fluorescence quenching nonlinearity relationship of $Cr^{3+}$.

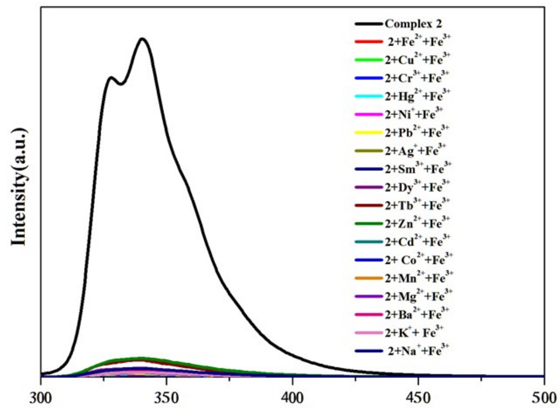



**Fig. S14.** Effect on the emission spectra of **2** dispersed in $H_2O$ upon incremental addition of $Fe^{3+}$ cations(1 mM) and the fluorescence quenching nonlinearity relationship of $Fe^{3+}$.

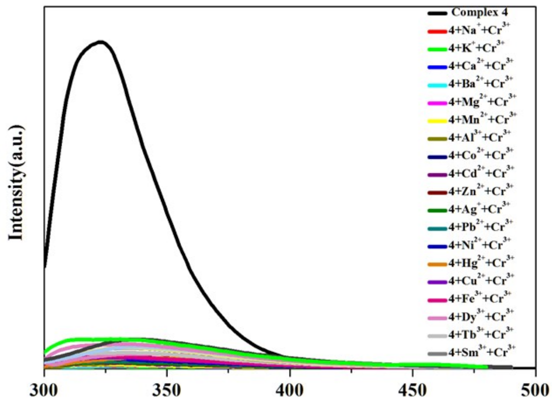



**Fig. S15.** Effect on the emission spectra of **4** dispersed in $H_2O$ upon incremental addition of $Cr^{3+}$ cations(1 mM) and the fluorescence quenching nonlinearity relationship of $Cr^{3+}$.

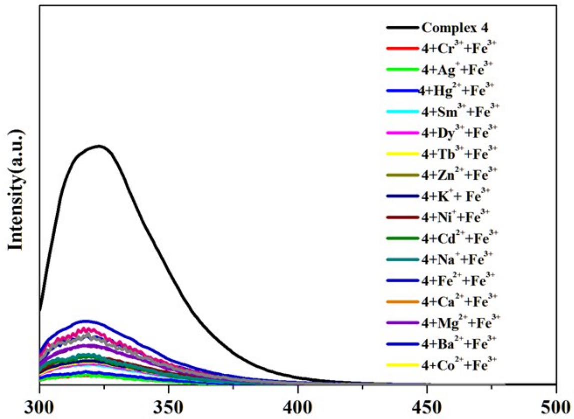



**Fig. S16.** Effect on the emission spectra of **4** dispersed in $H_2O$ upon incremental addition of $Fe^{3+}$ cations(1 mM) and the fluorescence quenching nonlinearity relationship of $Fe^{3+}$.

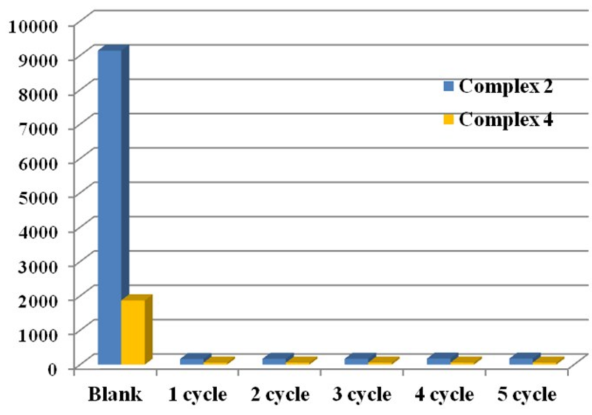



**Fig. S17.** Quenching rate histograms of **2** and **4** for sensing $Cr^{3+}$ caions up to five cycles.

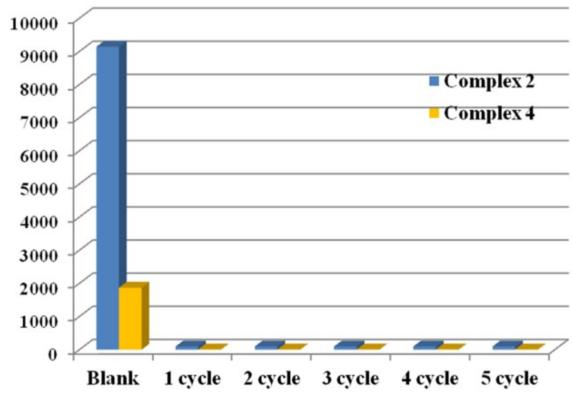



**Fig. S18.** Quenching rate histograms of **2** and **4** for sensing $Fe^{3+}$ caions up to five cycles.

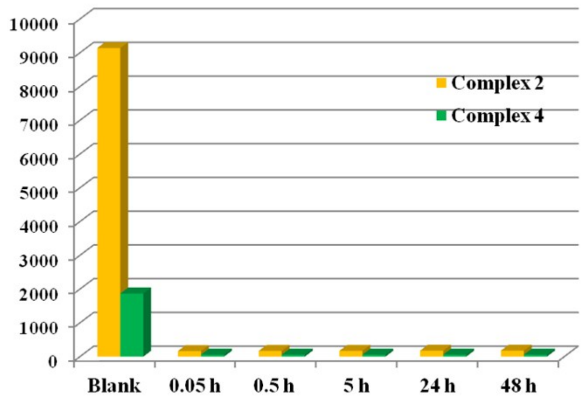



**Fig. S19.** The response time of **2** and **4** towards $Cr^{3+}$ (0.01 mol $L^{-1}$).

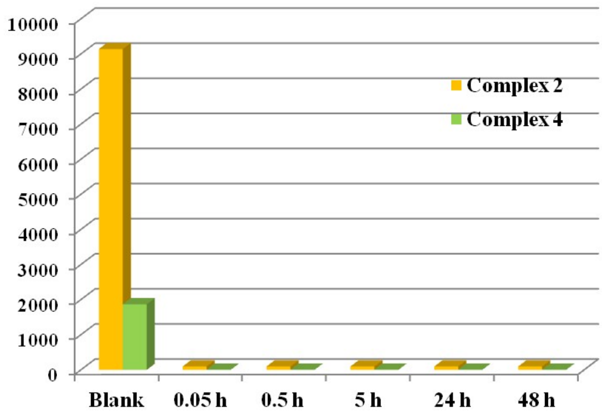



**Fig. S20.** The response time of **2** and **4** towards $Fe^{3+}$(0.01 mol $L^{-1}$).

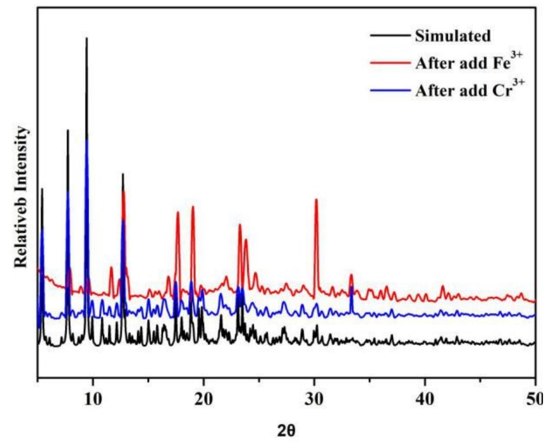



**Fig. S21**. The PXRD pattern of **2** after immerging in **$Fe^{3+}$ / $Cr^{3+}$.**

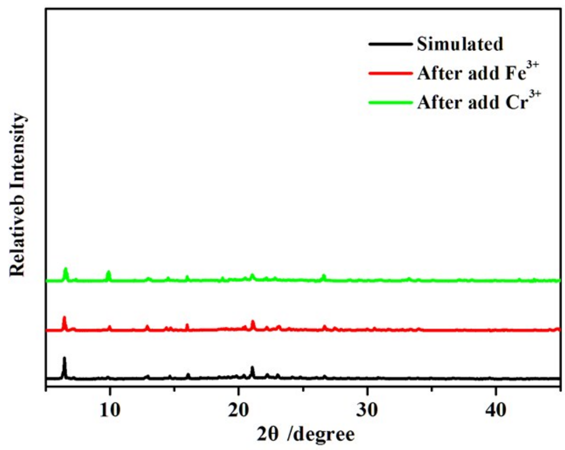



**Fig. S22**. The PXRD pattern of **4** after immerging in $Fe^{3+}$/$Cr^{3+}$.

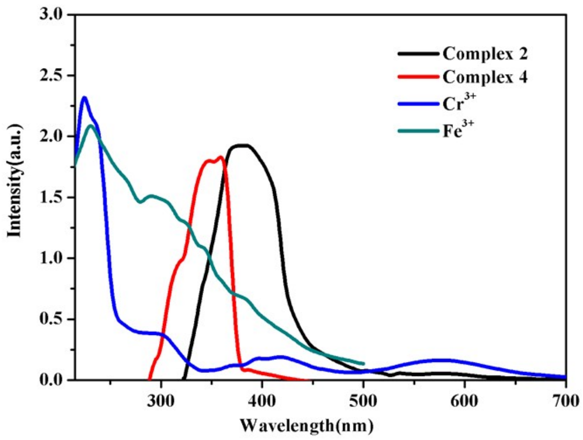



**Fig. S23.** Spectral overlap between the normalized emission spectrum of **2** and **4** and normalized absorption spectra of the $Cr^{3+}$ and $Fe^{3+}$.