# Syntheses, structures and luminescence properties of five coordination polymers based on designed 2,7-bis(4-benzoic acid)-N-(4-benzoic acid) carbazole

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**Table S1.** Selected bond lengths (Å) and angles (deg) for **TCZ-001 - TCZ-005**

| **TCZ-001** | | | |
|---|---|---|---|
| Zn(1)-O(4)#1 | 1.926(3) | Zn(2)-O(2) | 2.193(3) |
| Zn(1)-O(6) | 1.929(3) | Zn(3)-O(5) | 2.056(3) |
| Zn(1)-O(8) | 1.941(3) | Zn(3)-O(3)#1 | 2.058(3) |
| Zn(1)-O(16) | 2.009(3) | Zn(3)-O(13) | 2.087(3) |
| Zn(2)-O(11)#2 | 1.983(3) | Zn(3)-O(15) | 2.103(3) |
| Zn(2)-O(17) | 2.016(3) | Zn(3)-O(7) | 2.109(3) |
| Zn(2)-O(10) | 2.021(3) | Zn(3)-O(14) | 2.158(3) |
| Zn(2)-O(1) | 2.150(3) | | |
| O(4)#1-Zn(1)-O(6) | 129.39(13) | O(5)-Zn(3)-O(3)#1 | 96.61(11) |
| O(4)#1-Zn(1)-O(8) | 111.66(14) | O(5)-Zn(3)-O(13) | 85.66(11) |
| O(6)-Zn(1)-O(8) | 106.95(13) | O(3)#1-Zn(3)-O(13) | 172.02(11) |
| O(4)#1-Zn(1)-O(16) | 97.73(15) | O(5)-Zn(3)-O(15) | 93.14(12) |
| O(6)-Zn(1)-O(16) | 103.95(13) | O(3)#1-Zn(3)-O(15) | 85.68(12) |
| O(8)-Zn(1)-O(16) | 103.34(14) | O(13)-Zn(3)-O(15) | 86.56(11) |
| O(11)#2-Zn(2)-O(17) | 97.24(16) | O(5)-Zn(3)-O(7) | 96.66(12) |
| O(11)#2-Zn(2)-O(10) | 111.91(13) | O(3)#1-Zn(3)-O(7) | 96.36(12) |
| O(17)-Zn(2)-O(10) | 104.52(14) | O(13)-Zn(3)-O(7) | 90.96(12) |
| O(11)#2-Zn(2)-O(1) | 97.44(13) | O(15)-Zn(3)-O(7) | 169.68(12) |
| O(17)-Zn(2)-O(1) | 98.28(13) | O(5)-Zn(3)-O(14) | 176.55(11) |
| O(10)-Zn(2)-O(1) | 139.65(11) | O(3)#1-Zn(3)-O(14) | 86.72(11) |
| O(11)#2-Zn(2)-O(2) | 93.08(15) | O(13)-Zn(3)-O(14) | 91.16(11) |
| O(17)-Zn(2)-O(2) | 157.45(13) | O(15)-Zn(3)-O(14) | 87.99(11) |
| O(10)-Zn(2)-O(2) | 89.98(11) | O(7)-Zn(3)-O(14) | 82.04(11) |
| O(1)-Zn(2)-O(2) | 60.40(10) | | |

| **TCZ-002** |
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| | | | |
|---|---|---|---|
| Zn(1)-O(6) | 2.0198(17) | Zn(2)-O(3)#5 | 1.978(2) |
| Zn(1)-O(6)#1 | 2.0198(17) | Zn(2)-O(1)#3 | 1.984(2) |
| Zn(1)-O(2)#2 | 2.046(3) | Zn(2)-O(7) | 1.997(2) |
| Zn(1)-O(2)#3 | 2.046(3) | Zn(2)-O(3)#5 | 1.978(2) |
| Zn(1)-O(4)#4 | 2.094(2) | Zn(2)-O(1)#3 | 1.984(2) |
| Zn(1)-O(4)#5 | 2.094(2) | Zn(2)-O(7) | 1.997(2) |
| Zn(2)-O(5) | 1.9455(19) | | |
| O(6)-Zn(1)-O(6)#1 | 180.000(1) | O(6)#1-Zn(1)-O(4)#5 | 91.60(8) |
| O(6)-Zn(1)-O(2)#2 | 89.45(13) | O(2)#2-Zn(1)-O(4)#5 | 87.59(16) |
| O(6)#1-Zn(1)-O(2)#2 | 90.55(13) | O(2)#3-Zn(1)-O(4)#5 | 92.41(16) |
| O(6)-Zn(1)-O(2)#3 | 90.55(13) | O(4)#4-Zn(1)-O(4)#5 | 180.000(1) |
| O(6)#1-Zn(1)-O(2)#3 | 89.45(13) | O(5)-Zn(2)-O(3)#5 | 130.12(11) |
| O(2)#2-Zn(1)-O(2)#3 | 180.00(9) | O(5)-Zn(2)-O(1)#3 | 117.99(10) |
| O(6)-Zn(1)-O(4)#4 | 91.60(8) | O(3)#5-Zn(2)-O(1)#3 | 105.20(11) |
| O(6)#1-Zn(1)-O(4)#4 | 88.40(8) | O(5)-Zn(2)-O(7) | 97.49(10) |
| O(2)#2-Zn(1)-O(4)#4 | 92.41(16) | O(3)#5-Zn(2)-O(7) | 101.62(12) |
| O(2)#3-Zn(1)-O(4)#4 | 87.59(16) | O(1)#3-Zn(2)-O(7) | 96.22(12) |
| O(6)-Zn(1)-O(4)#5 | 88.40(8) | | |

**TCZ-003**

| | | | |
|---|---|---|---|
| Zn(1)-O(5)#1 | 1.933(4) | Zn(2)-O(15) | 1.982(3) |
| Zn(1)-O(3) | 1.942(4) | Zn(3)-O(9) | 1.981(3) |
| Zn(1)-O(7)#2 | 1.960(4) | Zn(3)-O(14) | 2.024(4) |
| Zn(1)-O(13) | 1.980(4) | Zn(3)-O(4) | 2.027(4) |
| Zn(2)-O(11)#1 | 1.941(3) | Zn(3)-O(12)#1 | 2.031(3) |
| Zn(2)-O(10) | 1.959(3) | Zn(3)-O(2)#2 | 2.049(4) |
| Zn(2)-O(1)#2 | 1.981(4) | | |
| O(5)#1-Zn(1)-O(3) | 126.33(16) | O(1)#2-Zn(2)-O(15) | 99.75(15) |
| O(5)#1-Zn(1)-O(7)#2 | 107.54(16) | O(9)-Zn(3)-O(14) | 99.26(15) |
| O(3)-Zn(1)-O(7)#2 | 98.27(17) | O(9)-Zn(3)-O(4) | 109.33(15) |
| O(5)#1-Zn(1)-O(13) | 107.44(17) | O(14)-Zn(3)-O(4) | 84.00(16) |
| O(3)-Zn(1)-O(13) | 96.91(18) | O(9)-Zn(3)-O(12)#1 | 102.86(15) |
| O(7)#2-Zn(1)-O(13) | 121.52(17) | O(14)-Zn(3)-O(12)#1 | 87.14(15) |
| O(11)#1-Zn(2)-O(10) | 123.71(15) | O(4)-Zn(3)-O(12)#1 | 147.57(16) |
| O(11)#1-Zn(2)-O(1)#2 | 115.88(15) | O(9)-Zn(3)-O(2)#2 | 107.00(17) |
| O(10)-Zn(2)-O(1)#2 | 110.09(15) | O(14)-Zn(3)-O(2)#2 | 153.52(17) |
| O(11)#1-Zn(2)-O(15) | 101.70(14) | O(4)-Zn(3)-O(2)#2 | 84.21(16) |
| O(10)-Zn(2)-O(15) | 100.72(14) | O(12)#1-Zn(3)-O(2)#2 | 90.23(16) |

**TCZ-004**

| | | | |
|---|---|---|---|
| Cd(1)-O(7) | 2.235(3) | Cd(2)-O(5)#4 | 2.167(2) |
| Cd(1)-O(7)#1 | 2.235(3) | Cd(2)-O(8) | 2.278(3) |
| Cd(1)-O(6) | 2.274(2) | Cd(2)-O(1) | 2.306(3) |
| Cd(1)-O(6)#1 | 2.274(2) | Cd(2)-O(4)#5 | 2.342(2) |

| | | | |
|---|---|---|---|
| Cd(1)-O(4)#2 | 2.340(2) | Cd(2)-O(3)#5 | 2.347(2) |
| Cd(1)-O(4)#3 | 2.340(2) | Cd(2)-O(2) | 2.376(3) |
| O(7)-Cd(1)-O(7)#1 | 180.000(1) | O(5)#4-Cd(2)-O(8) | 84.21(11) |
| O(7)-Cd(1)-O(6) | 91.40(9) | O(5)#4-Cd(2)-O(1) | 101.93(10) |
| O(7)#1-Cd(1)-O(6) | 88.60(9) | O(8)-Cd(2)-O(1) | 88.11(10) |
| O(7)-Cd(1)-O(6)#1 | 88.60(9) | O(5)#4-Cd(2)-O(4)#5 | 101.95(9) |
| O(7)#1-Cd(1)-O(6)#1 | 91.40(9) | O(8)-Cd(2)-O(4)#5 | 108.41(10) |
| O(6)-Cd(1)-O(6)#1 | 180.00(13) | O(1)-Cd(2)-O(4)#5 | 152.13(9) |
| O(7)-Cd(1)-O(4)#2 | 90.18(10) | O(5)#4-Cd(2)-O(3)#5 | 157.48(9) |
| O(7)#1-Cd(1)-O(4)#2 | 89.82(10) | O(8)-Cd(2)-O(3)#5 | 100.21(10) |
| O(6)-Cd(1)-O(4)#2 | 87.28(9) | O(1)-Cd(2)-O(3)#5 | 100.28(10) |
| O(6)#1-Cd(1)-O(4)#2 | 92.72(9) | O(4)#5-Cd(2)-O(3)#5 | 55.63(8) |
| O(7)-Cd(1)-O(4)#3 | 89.82(10) | O(5)#4-Cd(2)-O(2) | 100.66(10) |
| O(7)#1-Cd(1)-O(4)#3 | 90.18(10) | O(8)-Cd(2)-O(2) | 144.11(9) |
| O(6)-Cd(1)-O(4)#3 | 92.72(9) | O(1)-Cd(2)-O(2) | 56.02(9) |
| O(6)#1-Cd(1)-O(4)#3 | 87.28(9) | O(4)#5-Cd(2)-O(2) | 105.30(9) |
| O(4)#2-Cd(1)-O(4)#3 | 180.00(11) | O(3)#5-Cd(2)-O(2) | 88.70(10) |

| **TCZ-005** | | | |
|---|---|---|---|
| Cd(3)-O(2) | 2.287(4) | Cd(1)-O(42) | 2.213(5) |
| Cd(3)-O(9) | 2.292(5) | Cd(1)-O(21)#2 | 2.223(4) |
| Cd(3)-N(27) | 2.296(5) | Cd(1)-O(41) | 2.281(5) |
| Cd(3)-O(11)#1 | 2.346(5) | Cd(1)-O(14) | 2.316(5) |
| Cd(3)-O(12)#1 | 2.445(4) | Cd(2)-O(40) | 2.222(4) |
| Cd(3)-O(1) | 2.501(5) | Cd(2)-O(18) | 2.238(5) |
| Cd(3)-O(10) | 2.631(6) | Cd(2)-O(39) | 2.277(5) |
| Cd(4)-O(35)#2 | 2.283(5) | Cd(2)-O(16)#1 | 2.295(5) |
| Cd(4)-O(26) | 2.291(4) | Cd(2)-O(19) | 2.381(4) |
| Cd(4)-N(50) | 2.321(5) | Cd(2)-O(20) | 2.406(5) |
| Cd(4)-O(34) | 2.324(5) | Cd(5)-O(17) | 2.169(4) |
| Cd(4)-O(33) | 2.444(4) | Cd(5)-O(38) | 2.205(4) |
| Cd(4)-O(25) | 2.574(5) | Cd(5)-O(15)#1 | 2.214(4) |
| Cd(6)-O(45) | 2.247(7) | Cd(5)-O(37) | 2.275(5) |
| Cd(6)-O(29) | 2.318(5) | Cd(5)-O(19) | 2.331(5) |
| Cd(6)-O(28)#1 | 2.343(5) | Cd(8)-O(43) | 2.222(4) |
| Cd(6)-O(32) | 2.352(5) | Cd(8)-O(24) | 2.241(4) |
| Cd(6)-O(31) | 2.368(5) | Cd(8)-O(44) | 2.268(5) |
| Cd(6)-O(30) | 2.375(5) | Cd(8)-O(22)#2 | 2.280(5) |
| Cd(6)-O(27)#1 | 2.378(5) | Cd(8)-O(13) | 2.389(4) |
| Cd(7)-O(5)#1 | 2.232(6) | Cd(8)-O(14) | 2.391(4) |
| Cd(7)-O(46) | 2.313(7) | Cd(0A)-O(59) | 2.252(6) |
| Cd(7)-O(3) | 2.337(7) | Cd(0A)-O(6BA) | 2.269(5) |
| Cd(7)-O(8)#1 | 2.337(5) | Cd(0A)-O(58) | 2.281(6) |
| Cd(7)-O(4) | 2.425(7) | Cd(0A)-O(60) | 2.293(5) |

| | | | |
|---|---|---|---|
| Cd(7)-O(7)#1 | 2.445(5) | Cd(0A)-N(25) | 2.295(7) |
| Cd(7)-O(6)#1 | 2.489(7) | Cd(0A)-O(61) | 2.314(6) |
| Cd(1)-O(23) | 2.182(4) | | |
| O(2)-Cd(3)-O(9) | 99.82(17) | O(45)-Cd(6)-O(32) | 171.0(3) |
| O(2)-Cd(3)-N(27) | 160.1(2) | O(29)-Cd(6)-O(32) | 98.0(2) |
| O(9)-Cd(3)-N(27) | 89.23(19) | O(28)#1-Cd(6)-O(32) | 90.12(19) |
| O(2)-Cd(3)-O(11)#1 | 90.98(16) | O(45)-Cd(6)-O(31) | 116.2(3) |
| O(9)-Cd(3)-O(11)#1 | 132.45(18) | O(29)-Cd(6)-O(31) | 82.82(17) |
| N(27)-Cd(3)-O(11)#1 | 95.96(19) | O(28)#1-Cd(6)-O(31) | 131.68(17) |
| O(2)-Cd(3)-O(12)#1 | 80.85(16) | O(32)-Cd(6)-O(31) | 55.52(18) |
| O(9)-Cd(3)-O(12)#1 | 173.15(19) | O(45)-Cd(6)-O(30) | 94.9(2) |
| N(27)-Cd(3)-O(12)#1 | 88.11(18) | O(29)-Cd(6)-O(30) | 56.32(17) |
| O(11)#1-Cd(3)-O(12)#1 | 54.17(16) | O(28)#1-Cd(6)-O(30) | 84.34(17) |
| O(2)-Cd(3)-O(1) | 54.25(16) | O(32)-Cd(6)-O(30) | 93.36(19) |
| O(9)-Cd(3)-O(1) | 79.97(17) | O(31)-Cd(6)-O(30) | 125.74(18) |
| N(27)-Cd(3)-O(1) | 110.92(19) | O(45)-Cd(6)-O(27)#1 | 84.7(3) |
| O(11)#1-Cd(3)-O(1) | 138.97(14) | O(29)-Cd(6)-O(27)#1 | 161.1(2) |
| O(12)#1-Cd(3)-O(1) | 95.10(16) | O(28)#1-Cd(6)-O(27)#1 | 55.77(19) |
| O(2)-Cd(3)-O(10) | 100.50(17) | O(32)-Cd(6)-O(27)#1 | 91.3(2) |
| O(9)-Cd(3)-O(10) | 52.41(18) | O(31)-Cd(6)-O(27)#1 | 89.00(18) |
| N(27)-Cd(3)-O(10) | 99.08(18) | O(30)-Cd(6)-O(27)#1 | 139.84(19) |
| O(11)#1-Cd(3)-O(10) | 80.15(16) | O(5)#1-Cd(7)-O(46) | 86.3(2) |
| O(12)#1-Cd(3)-O(10) | 134.30(16) | O(5)#1-Cd(7)-O(3) | 172.3(3) |
| O(1)-Cd(3)-O(10) | 122.99(16) | O(46)-Cd(7)-O(3) | 89.4(3) |
| O(35)#2-Cd(4)-O(26) | 95.75(19) | O(5)#1-Cd(7)-O(8)#1 | 93.4(2) |
| O(35)#2-Cd(4)-N(50) | 92.3(2) | O(46)-Cd(7)-O(8)#1 | 98.5(2) |
| O(26)-Cd(4)-N(50) | 160.0(2) | O(3)-Cd(7)-O(8)#1 | 81.0(3) |
| O(35)#2-Cd(4)-O(34) | 131.0(2) | O(5)#1-Cd(7)-O(4) | 133.9(2) |
| O(26)-Cd(4)-O(34) | 95.17(17) | O(46)-Cd(7)-O(4) | 114.5(3) |
| N(50)-Cd(4)-O(34) | 93.24(19) | O(3)-Cd(7)-O(4) | 53.8(2) |
| O(35)#2-Cd(4)-O(33) | 174.1(2) | O(8)#1-Cd(7)-O(4) | 121.0(2) |
| O(26)-Cd(4)-O(33) | 83.72(17) | O(5)#1-Cd(7)-O(7)#1 | 87.8(2) |
| N(50)-Cd(4)-O(33) | 86.36(18) | O(46)-Cd(7)-O(7)#1 | 152.4(2) |
| O(34)-Cd(4)-O(33) | 54.93(17) | O(3)-Cd(7)-O(7)#1 | 93.2(3) |
| O(35)#2-Cd(4)-O(25) | 81.77(18) | O(8)#1-Cd(7)-O(7)#1 | 54.95(18) |
| O(26)-Cd(4)-O(25) | 53.51(16) | O(4)-Cd(7)-O(7)#1 | 88.6(2) |
| N(50)-Cd(4)-O(25) | 110.03(19) | O(5)#1-Cd(7)-O(6)#1 | 55.1(2) |
| O(34)-Cd(4)-O(25) | 139.83(16) | O(46)-Cd(7)-O(6)#1 | 108.8(3) |
| O(33)-Cd(4)-O(25) | 93.23(16) | O(3)-Cd(7)-O(6)#1 | 132.5(2) |
| O(45)-Cd(6)-O(29) | 83.7(3) | O(8)#1-Cd(7)-O(6)#1 | 135.2(2) |
| O(45)-Cd(6)-O(28)#1 | 94.3(3) | O(4)-Cd(7)-O(6)#1 | 78.9(2) |
| O(29)-Cd(6)-O(28)#1 | 140.09(17) | O(7)#1-Cd(7)-O(6)#1 | 89.54(19) |

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z-1; #2 x-

1,y,z+1 for **TCZ-001**;#1 -x+3/2,-y+3/2,-z+1;#2 x,-y+1,z-1/2;#3 -x+3/2,y+1/2,-z+3/2;#4 -x+2,-y+1,-z+2#5 x-1/2,y+1/2,z-1; #6 -x+3/2,y-1/2,-z+3/2; #7 x+1/2,y-1/2,z+1 for **TCZ-002**; #1 x-1,y-1,z-1;#2 -x,-y+1,-z+1; #3 x+1,y+1,z+1 for **TCZ-003**; #1 -x-2,-y,-z+3; #2 x-2,y,z+1; #3 -x,-y,-z+2; #4 -x-1,-y+1,-z+2; #5 -x+1,-y+1,-z+1; #6 x+2,y,z-1 for **TCZ-004**; #1 x,y+1,z; #2 x,y-1,z for **TCZ-005**

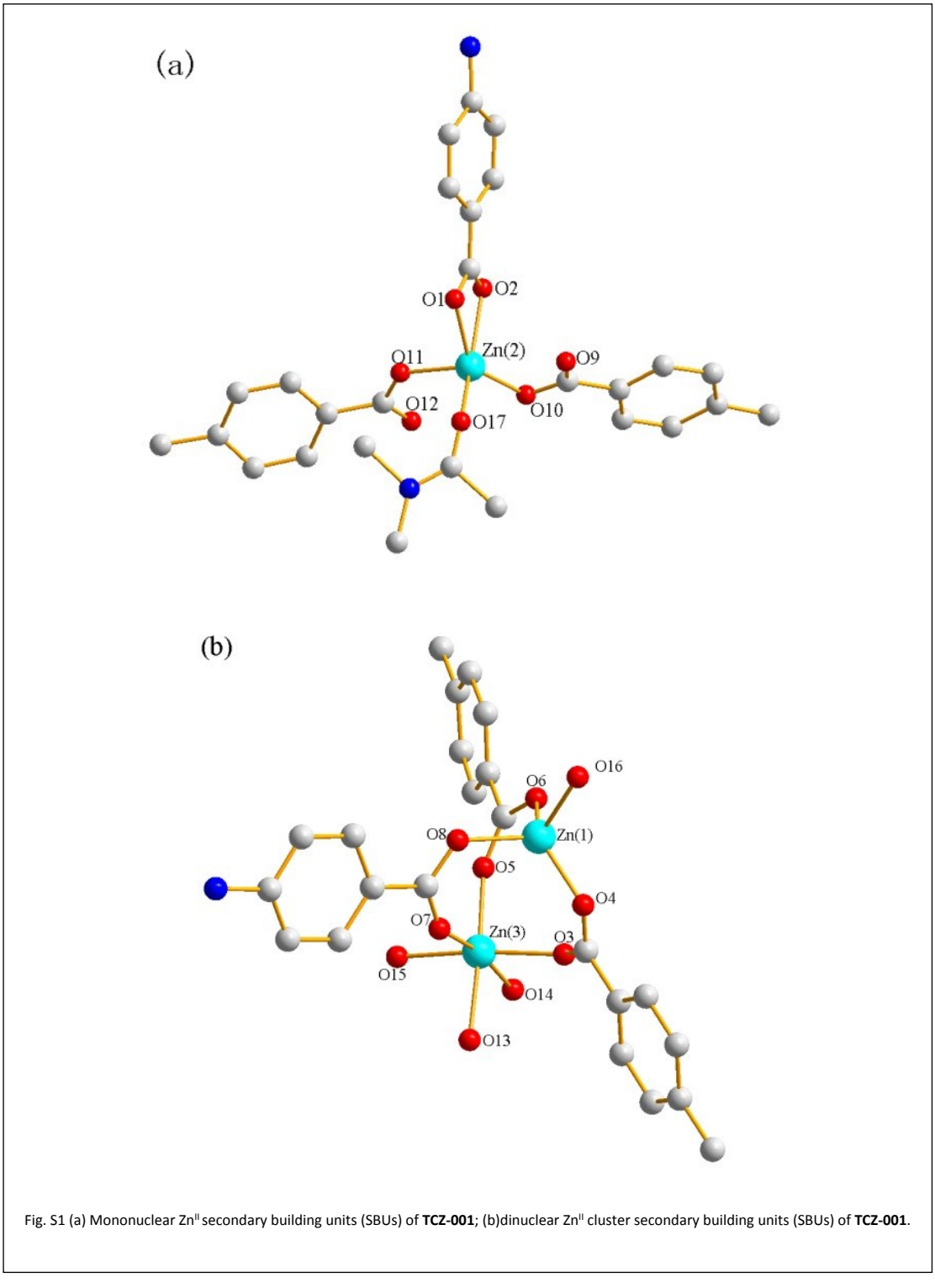



Fig. S1 (a) Mononuclear $Zn^{II}$ secondary building units (SBUs) of **TCZ-001**; (b)dinuclear $Zn^{II}$ cluster secondary building units (SBUs) of **TCZ-001**.

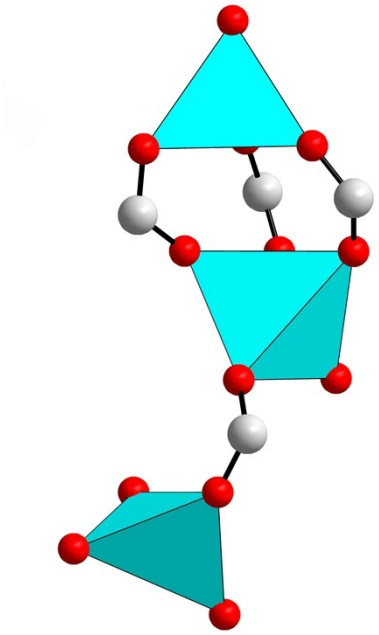


Fig. S2 Secondary building units (SBUs) of **TCZ-003**.

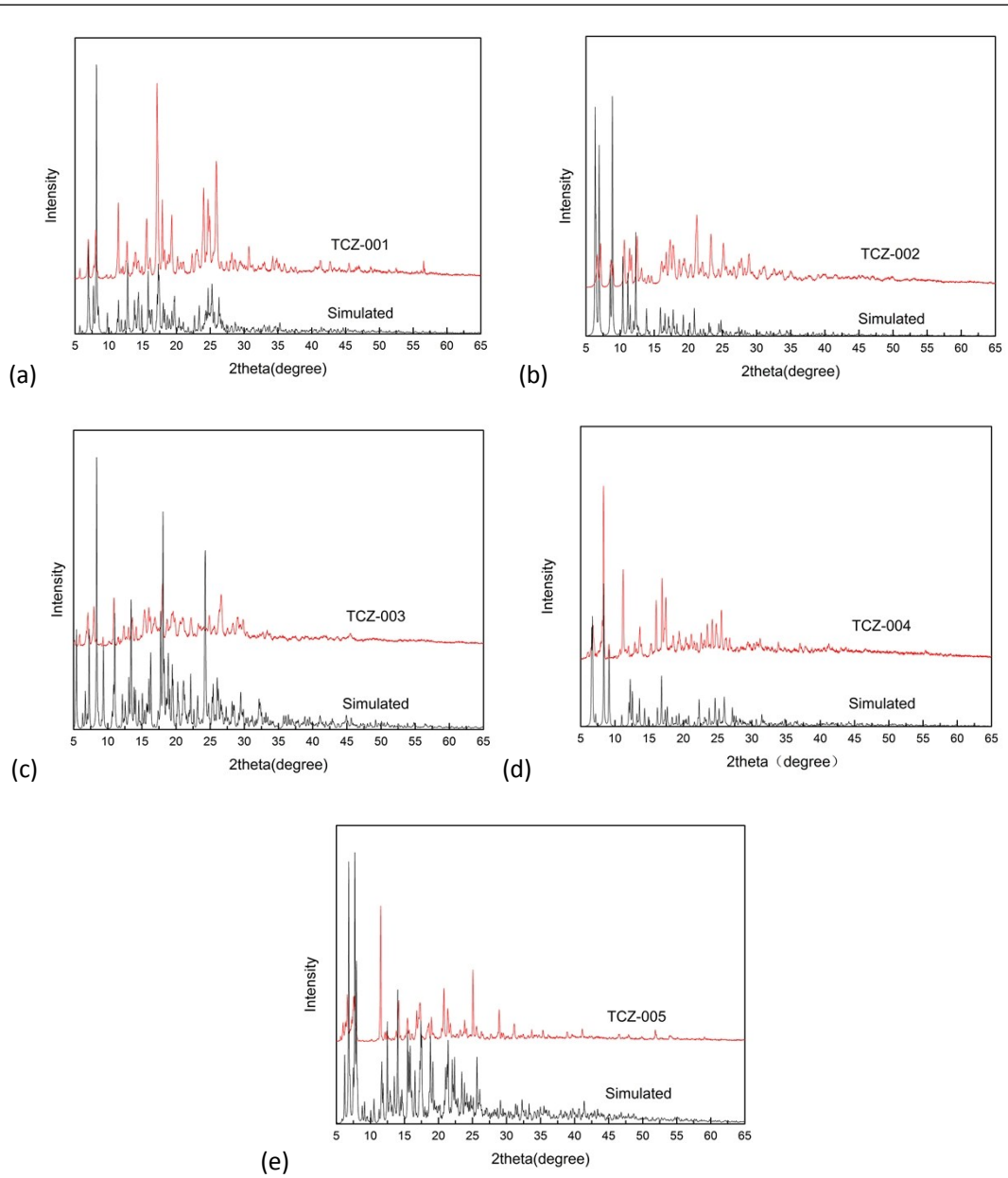



Fig. S3. Simulated (black), experimental (red) powder X-ray diffraction (PXRD) patterns for **TCZ-001**, **TCZ-002**, **TCZ-003**, **TCZ-004**, **TCZ-005**.

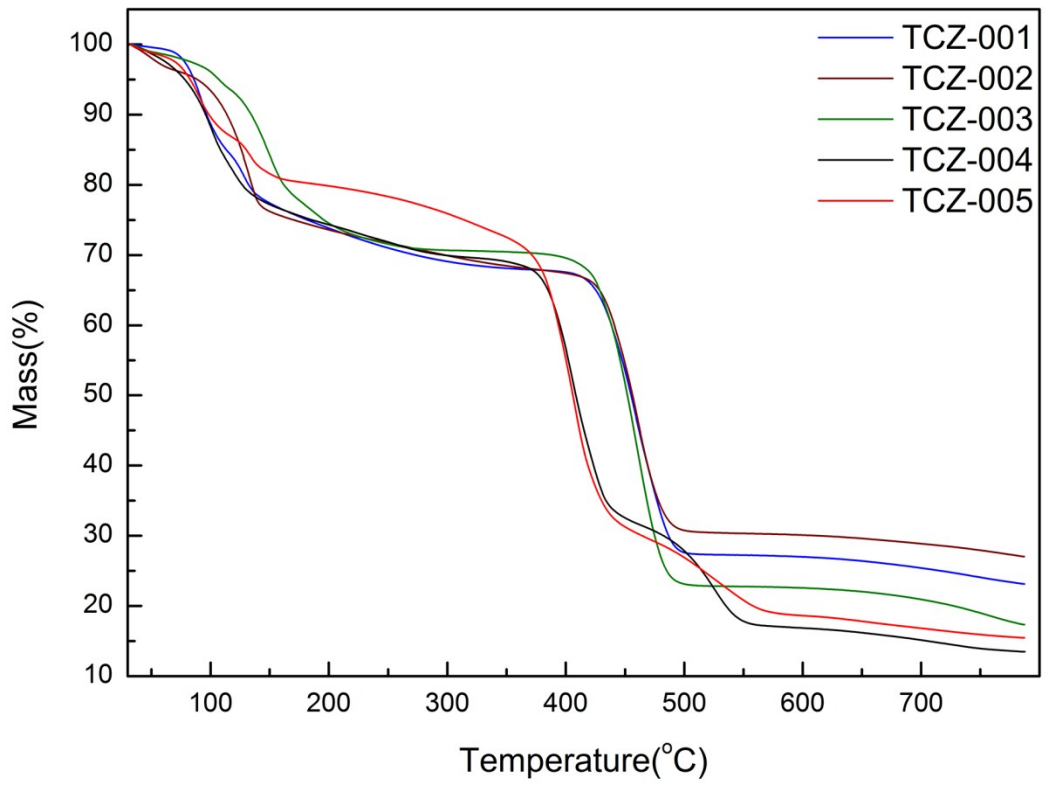



Fig. S4. Thermogravimetric analysis curves for **TCZ-001**, **TCZ-002**, **TCZ-003**, **TCZ-004** and **TCZ-005**.

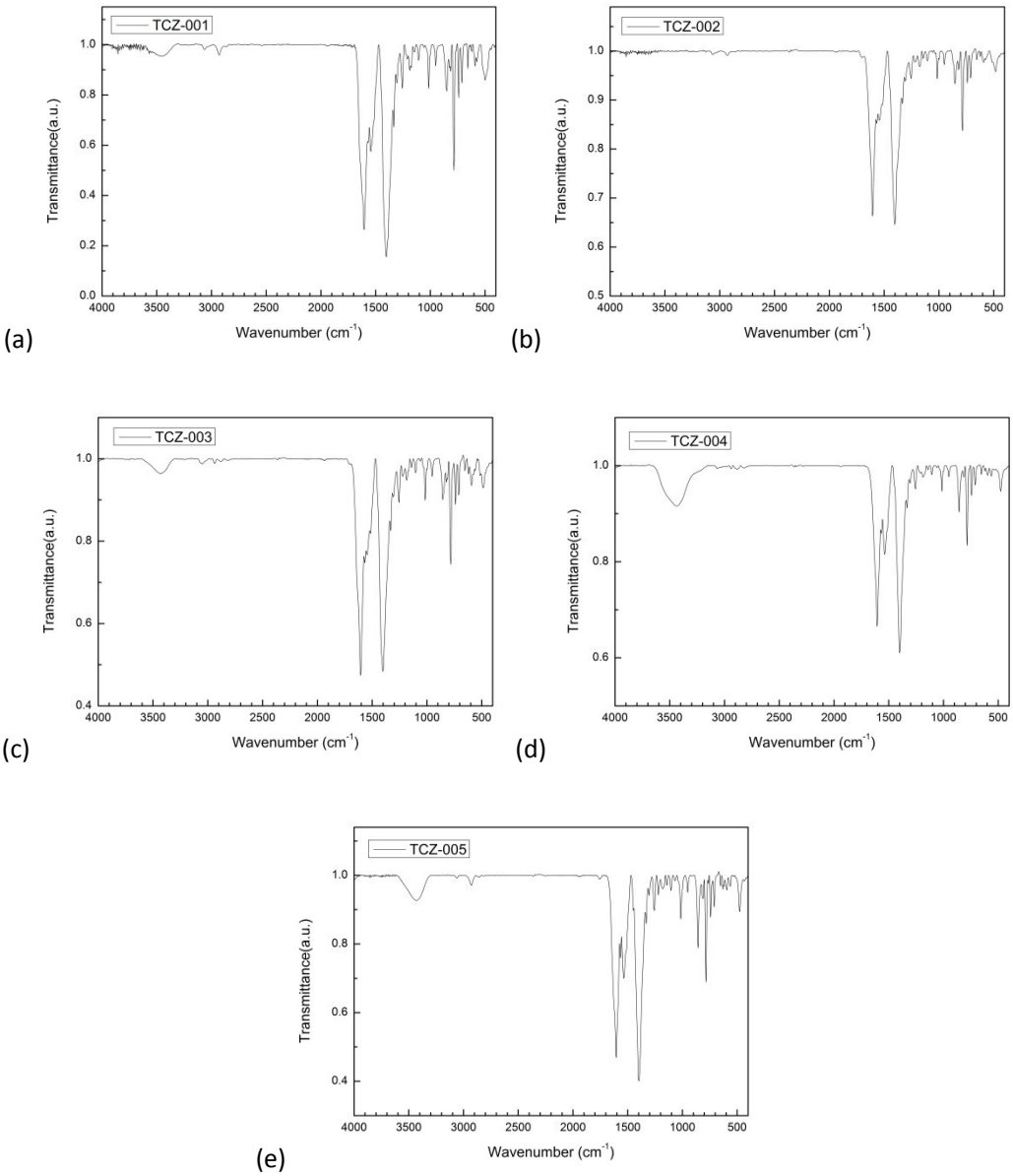



Fig. S5. Infrared spectra after baseline normalization for (a) **TCZ-001**, (b) **TCZ-002**, (c) **TCZ-003**, (d) **TCZ-004**, (e) **TCZ-005**. (KBr, $cm^{-1}$)

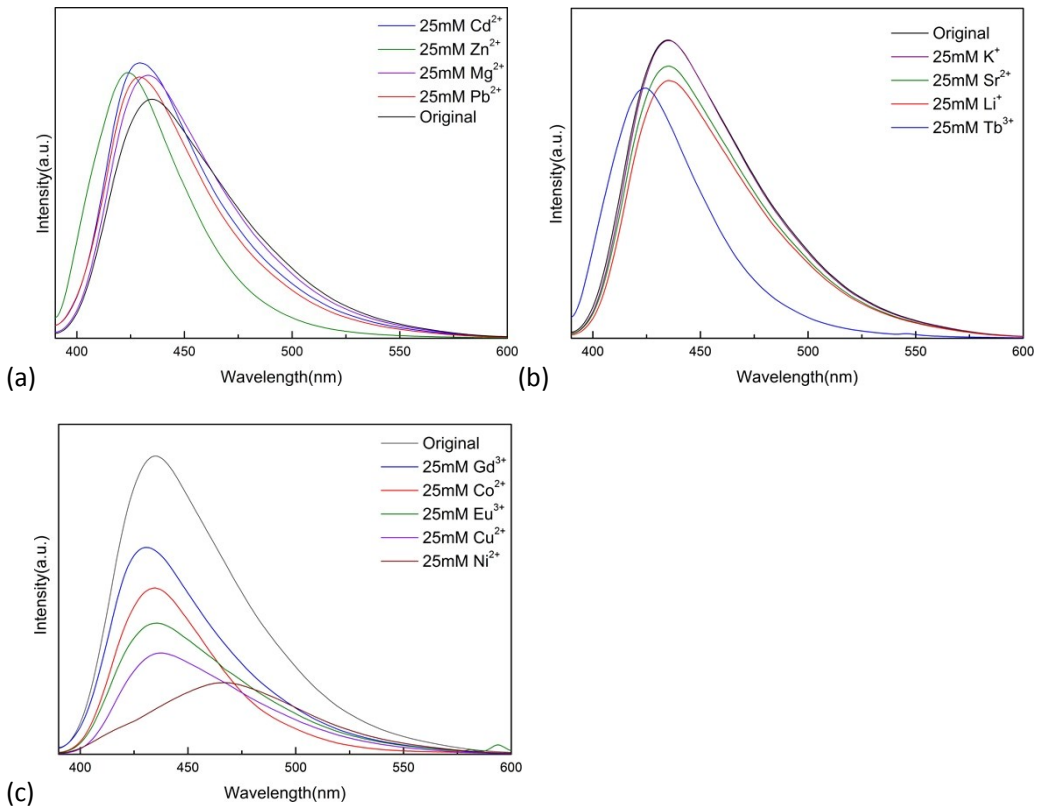



**Fig. S6** (a), (b) and (c)Emission spectra of TCZ-001 in DMA solution of diverse metal ions under excitation at 370nm.

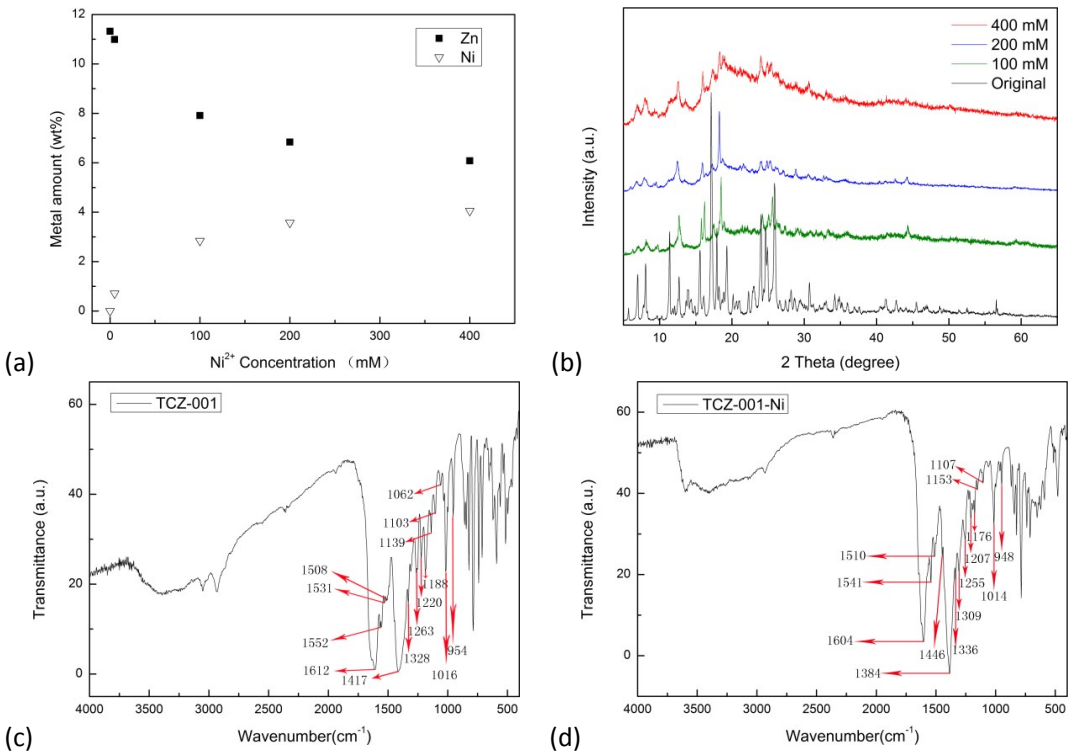
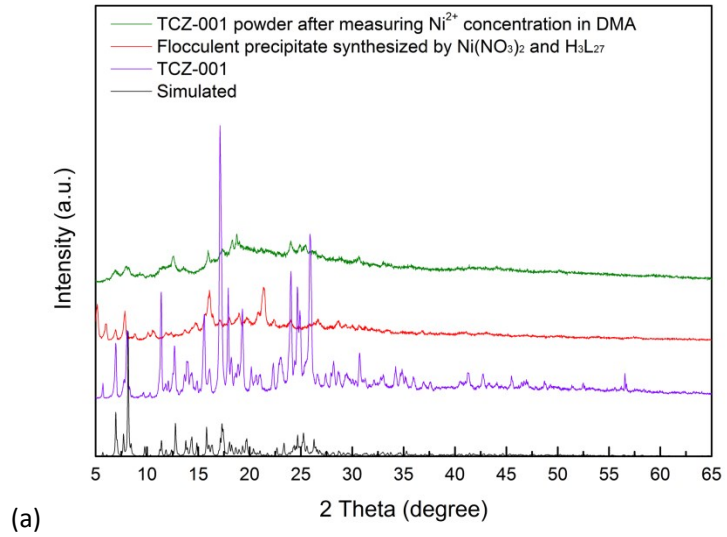
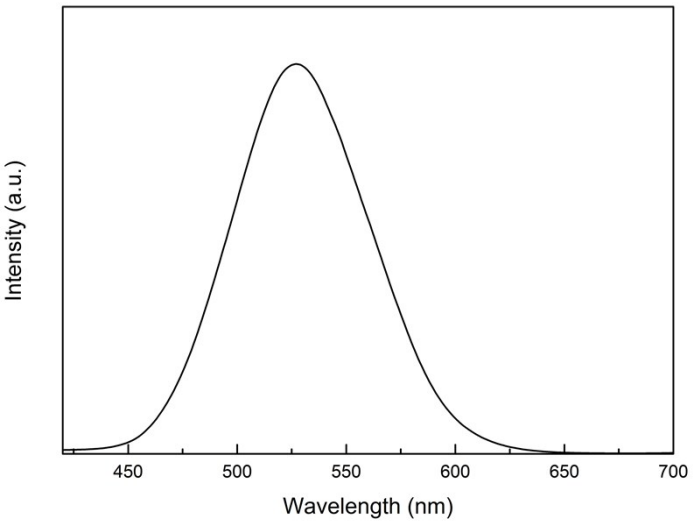



**Fig. S7** (a) Metal elemental weight (%) of the **TCZ-001** powders after measurements in different $Ni^{2+}$ concentrations in DMA solution; (b)PXRD patterns of the **TCZ-001** powders after measurements in different $Ni^{2+}$ concentrations in DMA solution; (c) Infrared spectra for TCZ-001 and (d) Infrared spectra for the **TCZ-001** powders after measurement.

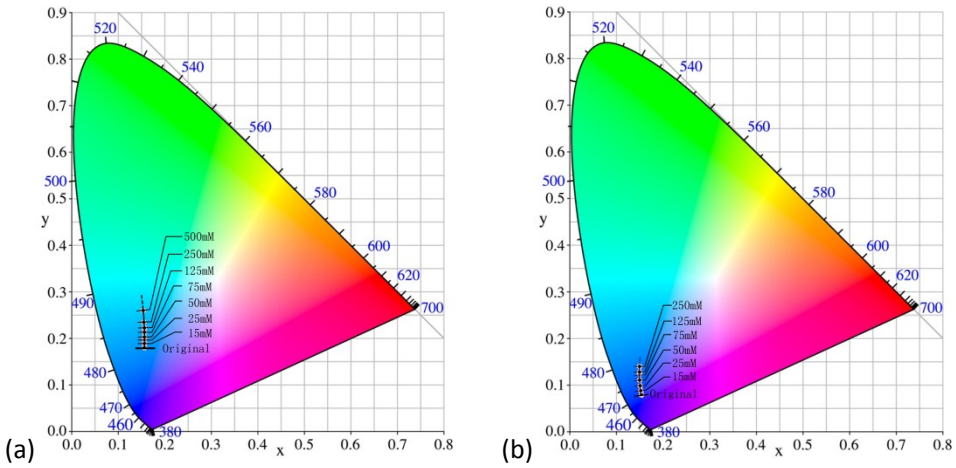



(a)




(b)

**Fig. S8** (a)Comparison of PXRD pattern between flocculent precipitate and TCZ-001; (b) solid-state emission of the flocculent precipitate.




(a)




(b)

**Fig. S9** (a) The relationship of luminescence colour of TCZ-001 and $Ni^{2+}$ concentration in $H_2O$; (b) The relationship of luminescence colour of TCZ-001 and $Ni^{2+}$ concentration in EtOH.

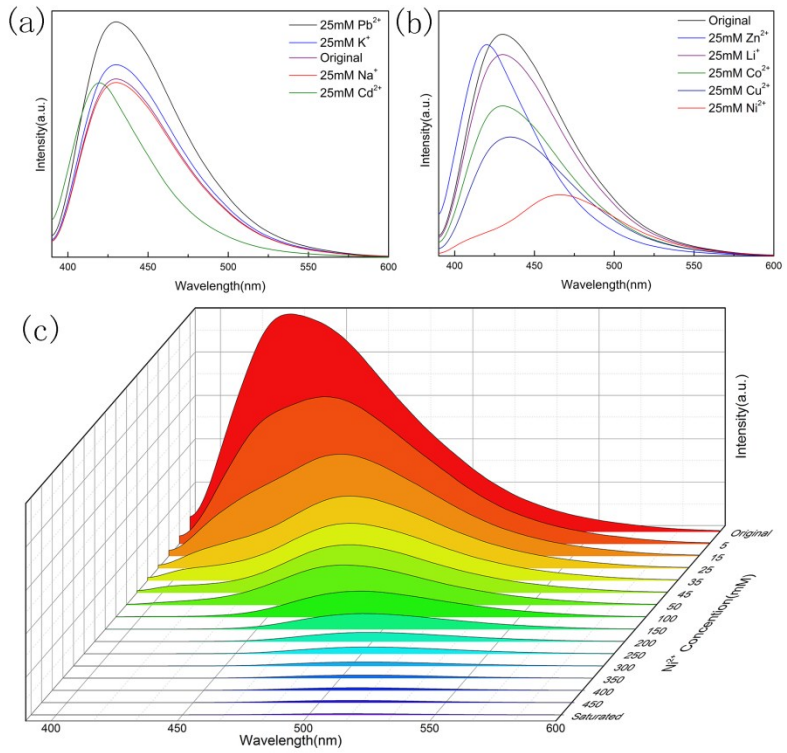



**Fig. S10** (a) and (b) Emission spectra of **TCZ-003** in DMA solution of diverse metal ions under excitation at 370 nm showing the selective sensing of $Ni^{2+}$; (c) Emission spectra of **TCZ-003** in DMA solution upon the addition of various concentrations of $Ni^{2+}$.

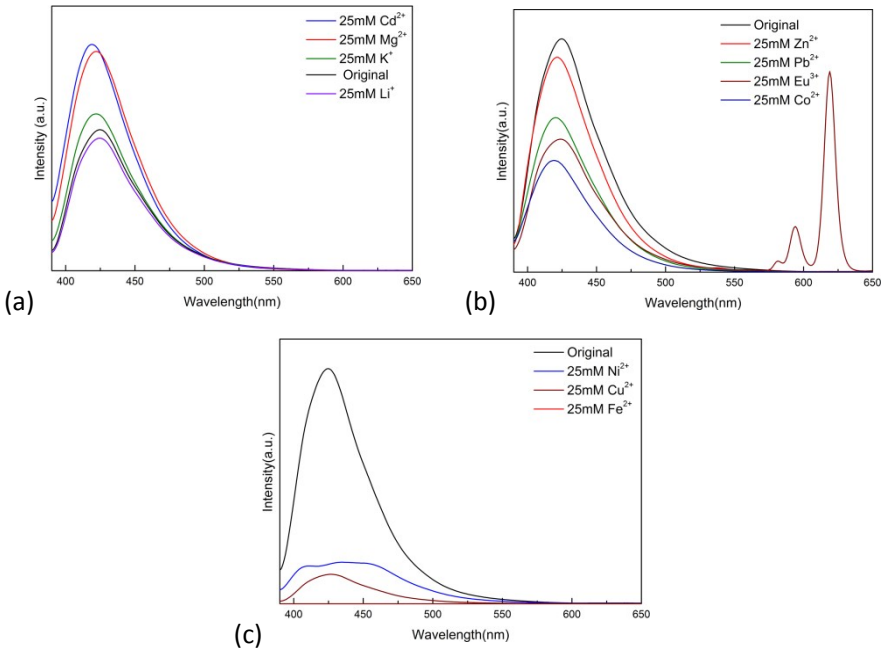



**Fig. S11** (a-c) Emission spectra of **TCZ-004** in DMA solution of diverse metal ions under excitation at 370nm.

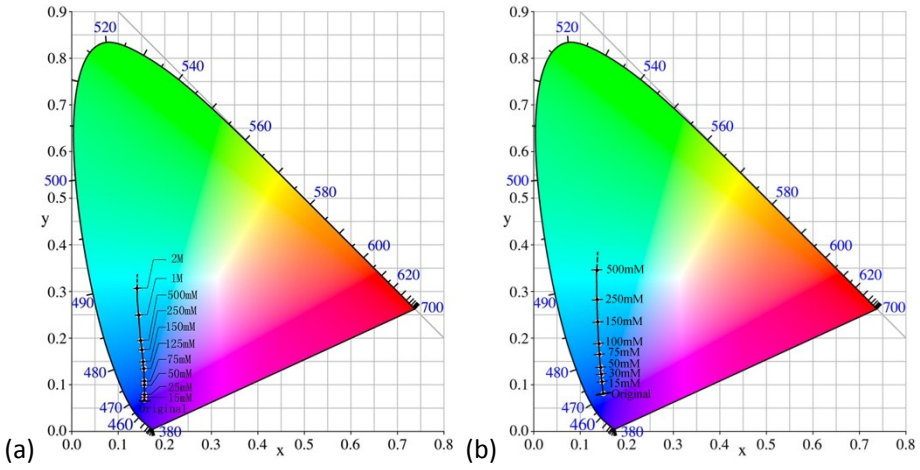



**Fig. S12** (a) The relationship of luminescence color of TCZ-004 and $Ni^{2+}$ concentration in $H_2O$; (b) The relationship of luminescence color of TCZ-004 and $Ni^{2+}$ concentration in EtOH.

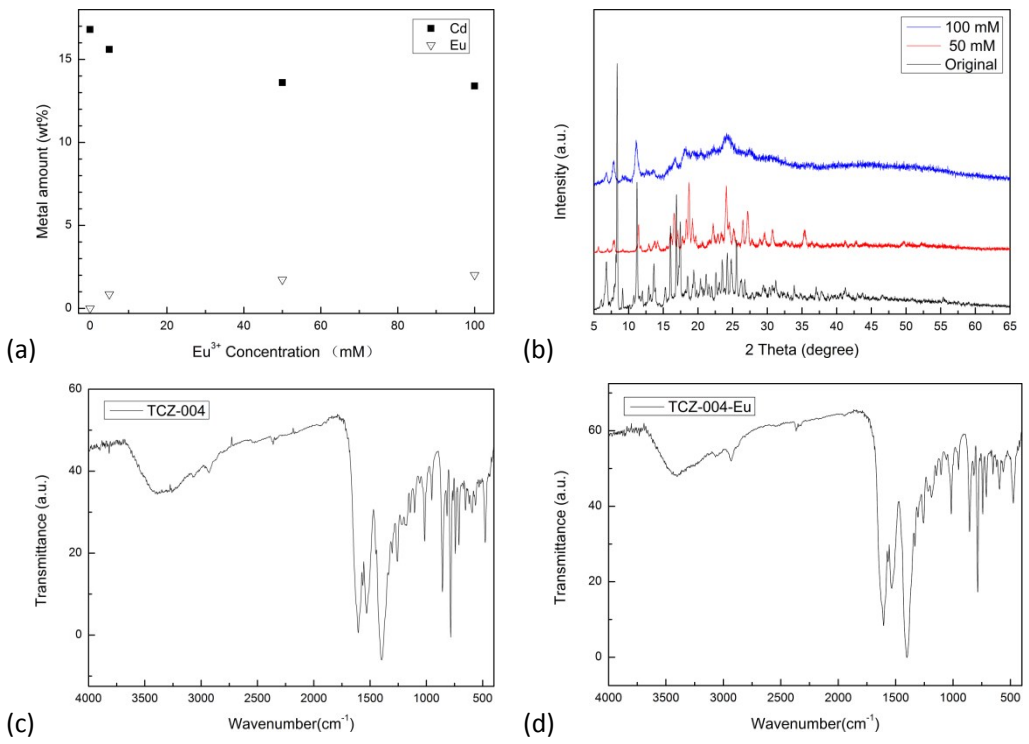



**Fig. S13** (a) Metal elemental weight (%) of the powders after measurements in different $Eu^{3+}$ concentrations in DMA solution; (b)PXRD patterns of the powders after measurements in different $Eu^{3+}$ concentrations in DMA solution; (c) Infrared spectra for TCZ-004 and (d) Infrared spectra for the powders after measurement.