Electronic Supplementary Material (ESI) for CrystEngComm. This journal is © The Royal Society of Chemistry 2019

Supporting Information

| Table S1. | Selected bond distances /Å and bond angles /° for 1-6 | | |
|------------|---|------------|------------|
| 1 | | | |
| Zn1-O8 | 1.998 (3) | Zn1-O2 | 2.005(3) |
| Zn1-N2 | 2.098(3) | Zn1-O1 | 2.441(3) |
| Zn1-N1 | 2.095(4) | Zn1-O9 | 2.455(3) |
| Zn2-O6 | 2.003(3) | Zn2-O10 | 2.045(3) |
| Zn2-O4 | 2.089(3) | Zn2-N4 | 2.112(3) |
| Zn2-N3 | 2.152(4) | Zn2-O3 | 2.417(3) |
| O8-Zn1-O2 | 121.84(11) | O8-Zn1-N2 | 113.32(11) |
| O2-Zn1-N2 | 109.84(12) | O8-Zn1-N1 | 109.71(12) |
| O2-Zn1-N1 | 116.07(12 | N2-Zn1-N 1 | 77.81(12) |
| O8-Zn1-O1 | 87.24(10) | O2-Zn1-O 1 | 58.52(10) |
| N2-Zn1-O1 | 86.34(11) | N1-Zn1-O1 | 160.27(11) |
| O8-Zn1-O9 | 57.93(10) | O2-Zn1-O9 | 90.18(10) |
| N2-Zn1-O9 | 158.71(11) | N1-Zn1-O9 | 87.02(12) |
| O1-Zn1-O9 | 111.16(10) | O6-Zn2-O10 | 93.39(11) |
| O6-Zn2-O4 | 98.50(11) | O10-Zn2-O4 | 99.36(12) |
| O6-Zn2-N4 | 103.50(12) | O10-Zn2-N4 | 90.94(12) |
| O4-Zn2-N4 | 155.08(11) | O6-Zn2-N3 | 91.99(11) |
| O10-Zn2-N3 | 167.10(12) | O4-Zn2-N3 | 91.41(12) |
| N4-Zn2-N3 | 76.39(12) | O6-Zn2-O3 | 156.39(10) |
| O10-Zn2-O3 | 93.06(10) | O4-Zn2-O3 | 58.02(9) |
| N4-Zn2-O3 | 99.08(10) | N3-Zn2-O3 | 86.62(10) |
| 2 | | | |
| Zn1-O7 | 1.966(2) | Zn2-O8 | 1.930(2) |
| Zn1-O10 | 2.006(3) | Zn2-O4 | 1.981(3) |
| Zn1-N2 | 2.100(3) | Zn2-N3 | 2.069(3) |
| Zn1-O1 | 2.107(3) | Zn2- N4 | 2.081(4) |
| Zn1-N1 | 2.220(3) | | |
| O7-Zn1-N2 | 122.14(11) | O10-Zn1-N2 | 106.56(12) |
| 07-Zn1-O1 | 92.28(11) | O10-Zn1-O1 | 90.32(11) |

| N2-Zn1-O1 | 88.27(12) | 07-Zn1-N1 | 95.53(11) |
|------------|------------|-----------|------------|
| O10-Zn1-N1 | 94.02(12) | N2-Zn1-N1 | 76.80(13) |
| O1-Zn1-N1 | 165.07(12) | O8-Zn2-O4 | 119.38(11) |
| O8-Zn2-N3 | 115.55(13) | O4-Zn2-N3 | 115.55(13) |
| O8-Zn2-N4 | 111.29(13) | O4-Zn2-N4 | 107.50(12) |
| N3-Zn2-N4 | 80.14(15) | | |
| 3 | | | |
| Cd1-N1 | 2.3112(19) | Cd1-O9 | 2.476(2) |
| Cd1-N2 | 2.333(2) | Cd1-O1 | 2.5407(15) |
| Cd1-O8 | 2.3555(15) | Cd1-O6 | 2.3938(16) |
| Cd1- O7 | 2.3953(16) | | |
| N1-Cd1-N2 | 71.18(7) | N1-Cd1-O1 | 81.40(6) |
| N1-Cd1-O8 | 155.64(6) | N2-Cd1-O1 | 138.18(7) |
| N2-Cd1- O8 | 121.25(6) | O8-Cd1-O1 | 76.13(5) |
| N1-Cd1-O6 | 89.53(6) | O6-Cd1-O1 | 77.58(5) |
| N2-Cd1-O6 | 131.37(6) | N2-Cd1-O1 | 138.18(7) |
| O8-Cd1-O6 | 94.67(5) | N1-Cd1-O1 | 81.40(6) |
| N1-Cd1-O7 | 109.61(6) | O8-Cd1-O1 | 76.13(5) |
| N2-Cd1-O7 | 89.25(7) | O6-Cd1-O1 | 77.58(5) |
| O8-Cd1-O7 | 92.26(5) | O7-Cd1-O1 | 130.31(5) |
| O6-Cd1-O7 | 55.06(5) | O9-Cd1-O1 | 83.31(8) |
| N1-Cd1-O9 | 114.63(7) | | |
| 4 | | | |
| Cd1-O1 | 2.3113(18) | Cd1-O3 | 2.2969(18) |
| Cd1-O4 | 2.290(2) | Cd1-O6 | 2.180(2) |
| Cd1-O8 | 2.3722(19) | Cd1-O9 | 2.369(18) |
| Cd2-O1 | 2.5994(19) | Cd2-O2 | 2.3242(18) |
| Cd2-O7 | 2.234(2) | Cd2-O8 | 2.3086(19) |
| Cd2-N1 | 2.307(2) | Cd2-N2 | 2.284(2) |
| O6-Cd1-O4 | 99.13(10) | O6-Cd1-O3 | 124.30(9) |
| O4-Cd1-O3 | 56.50(7) | O6-Cd1-O1 | 79.98(9) |
| O4-Cd1 -O1 | 151.53(8) | O3-Cd1-O1 | 100.30(7) |
| O6-Cd1-O9 | 138.41(9) | O4-Cd1-O9 | 106.82(10) |

| O3-Cd1-O9 | 97.22(8) | O1-Cd1-O9 | 91.18(9) |
|-------------|-----------|-------------|------------|
| O6-Cd1-O8 | 86.41(8) | O4-Cd1-O8 | 109.33(8) |
| O3-Cd1-O8 | 146.06(8) | O1-Cd1-O8 | 99.04(7) |
| O9-Cd1-O8 | 54.71(7) | O2-Cd2-O1 | 52.43(6) |
| O7-Cd2-N2 | 175.75(8) | 07-Cd2-N1 | 94.51(8) |
| N2-Cd2-N1 | 83.39(8) | O7-Cd2-O8 | 87.84(7) |
| N2-Cd2-O8 | 88.60(7) | N1-Cd2-O8 | 93.51(8) |
| O7-Cd2-O2 | 87.32(8) | N2-Cd2-O2 | 96.54(8) |
| N1-Cd2-O2 | 95.25(7) | O8-Cd2-O2 | 170.29 (7) |
| O7-Cd2-O1 | 88.13(8) | N2-Cd2-O1 | 95.63(8) |
| N1-Cd2-O1 | 147.46(7) | O8-Cd2-O1 | 119.02(7) |
| 5 | | | |
| Cd1-O10 | 2.208(2) | Cd3-O7 | 2.241(2) |
| Cd1-O19 | 2.227(2) | Cd3-O16 | 2.281(2) |
| Cd1-O1 | 2.327(2) | Cd3-O17 | 2.309(2) |
| Cd1-O4 | 2.339(2) | Cd3-O24 | 2.438(6) |
| Cd1-O3 | 2.397(2) | Cd3-O24A | 2.338(6) |
| Cd1-O20 | 2.434(3) | Cd3-O18 | 2.450(2) |
| Cd2-O9 | 2.209(2) | Cd4-O1 | 2.465(2) |
| Cd2-O11 | 2.234(2) | Cd4-O27 | 2.223(3) |
| Cd2-O6 | 2.263(2) | Cd4-O26 | 2.228(3) |
| Cd2-O23 | 2.264(2) | Cd4-O15 | 2.255(2) |
| Cd2-O21 | 2.283(2) | Cd4-O2 | 2.378(2) |
| Cd2-O22 | 2.505(3) | Cd4-O28 | 2.448(3) |
| Cd3-O25 | 2.212(2) | | |
| O10-Cd1-O1 | 99.77(8) | O10-Cd1-O19 | 125.90(9) |
| O10-Cd1-O4 | 138.92(8) | O19-Cd1-O1 | 83.36(8) |
| O1-Cd1-O4 | 94.11(8) | O19-Cd1-O4 | 93.87(9) |
| O19-Cd1-O3 | 142.35(9) | O10-Cd1-O3 | 84.43(8) |
| O4-Cd1-O3 | 54.87(8) | O1-Cd1-O3 | 115.95(9) |
| O19-Cd1-O20 | 79.62(9) | O10-Cd1-O20 | 85.07(9) |
| O4-Cd1-O20 | 93.58(9) | O1-Cd1-O20 | 161.75(8) |
| O9-Cd2-O11 | 107.54(8) | O3-Cd1-O20 | 81.90(10) |

| O11-Cd2-O6 | 93.94(8) | O9-Cd2-O6 | 90.44(8) |
|--------------|------------|--------------|------------|
| O11-Cd2-O23 | 102.17(9) | O9-Cd2-O23 | 150.23(8) |
| O9-Cd2-O21 | 93.08(9) | O6-Cd2-O23 | 85.62(8) |
| O6-Cd2-O21 | 172.05(8) | O11-Cd2-O21 | 91.79(9) |
| O9-Cd2-O22 | 70.57(9) | O23-Cd2-O21 | 87.79(9) |
| O6-Cd2-O22 | 84.37(8) | O11-Cd2-O22 | 177.42(9) |
| O21-Cd2-O22 | 90.08(9) | O23-Cd2-O22 | 79.68(9) |
| O25-Cd3-O16 | 83.33(9) | O25-Cd3-O7 | 118.82(9) |
| O25-Cd3-O17 | 152.20(10) | O7-Cd3-O16 | 107.98(9) |
| O16-Cd3-O17 | 100.86(10) | O7-Cd3-O17 | 86.31(8) |
| O7-Cd3-O24A | 90.52(15) | O25-Cd3-O24A | 84.70(15) |
| O17-Cd3-O24A | 83.32(16) | O16-Cd3-O24A | 161.18(15) |
| O7-Cd3-O24 | 98.18(15) | O25-Cd3-O24 | 74.52(15) |
| O17-Cd3-O24 | 91.24(15) | O16-Cd3-O24 | 151.69(14) |
| O25-Cd3-O18 | 100.44(9) | O24A-Cd3-O24 | 10.66(19) |
| O16-Cd3-O18 | 77.81(8) | O7-Cd3-O18 | 140.62(8) |
| O24A-Cd3-O18 | 90.16(16) | O17-Cd3-O18 | 54.71(8) |
| O27-Cd4-O26 | 99.30(12) | O24-Cd3-O18 | 88.93(15) |
| O26-Cd4-O15 | 97.82(10) | O27-Cd4-O15 | 129.96(9) |
| O26-Cd4-O2 | 104.09(10) | O27-Cd4-O2 | 137.66(9) |
| O27-Cd4-O28 | 84.29(11) | O15-Cd4-O2 | 81.14(7) |
| O15-Cd4-O28 | 81.62(9) | O26-Cd4-O28 | 175.62(11) |
| O27-Cd4-O1 | 93.64(8) | O2-Cd4-O28 | 71.53(10) |
| O15-Cd4-O1 | 133.99(7) | O26-Cd4-O1 | 86.97(8) |
| O28-Cd4-O1 | 90.31(9) | O2-Cd4-O1 | 53.58(7) |
| 6 | | | |
| Cd1-O4 | 2.247(2) | Cd1-N2 | 2.295(3) |
| Cd1-O1 | 2.398(2) | Cd1-N1 | 2.444(3) |
| Cd1-O2 | 2.455(2) | Cd1-O2#3 | 2.602(2) |
| Cd1-O3 | 2.614(2) | Cd2-N3 | 2.302(3) |
| Cd2-N4 | 2.329(3) | Cd2-O10 | 2.333(3) |
| Cd2-O6 | 2.409(2) | Cd2-O9 | 2.461(2) |
| Cd2-O8 | 2.490(2) | Cd2-07 | 2.555(2) |
| | | | |

| Cd2-O1 | 2.602(3) | | |
|------------|-----------|------------|-----------|
| O4-Cd1-O1 | 128.44(8) | O4-Cd1-N2 | 144.08(9) |
| O4-Cd1-N1 | 91.97(9) | N2-Cd1-O1 | 86.80(9) |
| O1-Cd1-N1 | 83.23(9) | N2-Cd1-N1 | 100.05(9) |
| N2-Cd1-O2 | 122.25(8) | O4-Cd1-O2 | 82.57(8) |
| N1-Cd1-O2 | 112.82(9) | O1-Cd2-O2 | 53.81(8) |
| N2-Cd1-O2 | 81.07(9) | O8-Cd2-O7 | 86.15(8) |
| N1-Cd1-O2 | 171.64(8) | O1-Cd1-O2 | 105.13(8) |
| O2-Cd1-O2 | 72.85(8) | N2-Cd1-O3 | 94.38(8) |
| O1-Cd1-O3 | 166.26(8) | N1-Cd1-O3 | 83.09(8) |
| O2-Cd1-O3 | 134.16(7) | O2-Cd1-O3 | 88.57(7) |
| N3-Cd2-N4 | 95.94(10) | N3-Cd2-O10 | 168.97(9) |
| N4-Cd2-O10 | 91.34(9) | N3-Cd2-O6 | 92.07(9) |
| N4-Cd2-O6 | 84.37(9) | O10-Cd2-O6 | 80.38(9) |
| N3-Cd2-O9 | 106.36(9) | N4-Cd2-O9 | 85.00(9) |
| O10-Cd2-O9 | 82.48(8) | O6-Cd2-O9 | 159.57(9) |
| N3-Cd2-O8 | 90.57(9) | N4-Cd2-O8 | 136.94(9) |
| O10-Cd2-O8 | 89.75(8) | O6-Cd2-O8 | 138.01(8) |
| O9-Cd2-O8 | 52.51(8) | N3-Cd2-O7 | 85.98(9) |
| N4-Cd2-O7 | 136.67(9) | O10-Cd2-O7 | 83.04(8) |
| O6-Cd2-O7 | 52.31(8) | O9-Cd2-O7 | 135.99(8) |

Symmetry codes for 1: A (-x, 1-y, 1-z), B (-1+x, y, 1+z); for 2: A (x, -1+y, -z), B (1-x, 2-y, -z); for 3: A (1+x, y, z), B (2-x, 1-y, -z); for 4: A (-1+x, y, z), B (1-x, 1-y, -z), C (2-x, -y, 1-z); for 5: A (1-x,1-y, -z), B (1-x,1-y, 1-z), C (-x, -y, 1-z), D (-1+x, -1+y, z), for 6: A (-1+x, y, z), B (1-x, 1-y, 1-z), C (x, -0.5-y, -0.5+z), D (-x, -y, 1-z).

Figure S1. Standard curve of zinc series.



Figure S2. Standard curve of cadmium series.

















Figure S5. The emission spectra of 2 introduced into various pure organic solvents excited at 280 nm.

