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# Supplementary Material

## Syntheses, photoluminescent properties and structural investigation of five complexes based on a new T-Shaped 2-(pyridin-3-yl)-4,6-pyrimidine dicarboxylic acid ligand: structure evolution from one-dimensional chains to three-dimensional architectures

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**Table S1** Selected bond distances (Å) and angles (deg) for the complexes **1**–**5**[a]

| | | | | | |
|---|---|---|---|---|---|
| | | | Complex **1** | | |
| Mn(1)-O(4)$^{i}$ | 2.0950(19) | Mn(1)-O(5) | 2.140(2) | Mn(1)-N(1) | 2.384(2) |
| Mn(1)-O(6)$^{ii}$ | 2.124(2) | Mn(1)-O(1) | 2.1440(19) | Mn(1)-N(2)$^{i}$ | 2.458(2) |
| O(4)$^{i}$-Mn(1)-O(6) | 86.62(8) | O(5)-Mn(1)-O(1) | 90.54(7) | O(4)$^{i}$-Mn(1)-N(2)$^{i}$ | 72.85(7) |
| O(4)$^{i}$-Mn(1)-O(5) | 88.76(7) | O(4)$^{i}$-Mn(1)-N(1) | 111.41(7) | O(6)-Mn(1)-N(2)$^{i}$ | 154.87(8) |
| O(6)-Mn(1)-O(5) | 108.88(9) | O(6)-Mn(1)-N(1) | 94.90(8) | O(5)-Mn(1)-N(2)$^{i}$ | 85.49(7) |
| O(4)$^{i}$-Mn(1)-O(1) | 171.18(7) | O(5)-Mn(1)-N(1) | 149.89(7) | O(1)-Mn(1)-N(2)$^{i}$ | 115.86(7) |
| O(6)-Mn(1)-O(1) | 85.29(8) | O(1)-Mn(1)-N(1) | 72.84(7) | N(1)-Mn(1)-N(2)$^{i}$ | 79.86(7) |
| | | | Complex **2** | | |
| Cu(1)-O(1) | 1.9359(16) | Cu(1)-O(5) | 1.9671(17) | Cu(1)-N(1) | 2.6149(18) |
| Cu(1)-O(4)$^{i}$ | 1.9416(16) | Cu(1)-O(6) | 1.9601(16) | | |
| O(1)-Cu(1)-O(4)$^{i}$ | 179.52(6) | O(4)$^{i}$ -Cu(1)-O(5) | 89.96(7) | O(4)$^{i}$ -Cu(1)-N(1) | 106.28(6) |
| O(1)-Cu(1)-O(6) | 90.19(7) | O(6)-Cu(1)-O(5) | 177.59(7) | O(6)-Cu(1)-N(1) | 91.08(7) |
| O(4)$^{i}$ -Cu(1)-O(6) | 90.15(7) | O(1)-Cu(1)-N(1) | 176.29(8) | O(5)-Cu(1)-N(1) | 86.58(7) |
| O(1)-Cu(1)-O(5) | | | | | |
| | | | Complex **3** | | |
| Co(1)-O(1)$^{i}$ | 2.0392(15) | Co(1)-N(1)$^{i}$ | 2.2215(18) | Co(2)-N(2)$^{iv}$ | 2.2111(17) |
| Co(1)-N(3)$^{ii}$ | 2.2198(18) | Co(2)-O(4)$^{iv}$ | 2.0394(15) | Co(2)-O(4) | 2.0394(15) |
| Co(1)-N(3)$^{iii}$ | 2.2198(18) | Co(2)-N(2) | 2.2111(17) | Co(2)-O(5) | 2.0781(16) |
| Co(2)-O(5)$^{iv}$ | 2.0781(16) | Co(1)-N(1) | 2.2215(18) | Co(1)-O(1) | 2.0392(15) |
| O(1)$^{i}$-Co(1)-O(1) | 180.000(1) | N(3)$^{iii}$-Co(1)-N(1)$^{i}$ | 93.26(7) | O(5)$^{iv}$-Co(2)-O(5) | 180.000(1)) |
| O(1)$^{i}$-Co(1)-N(3)$^{ii}$ | 89.01(6) | O(1)-Co(1)-N(1) | 78.08(6) | O(4)-Co(2)-N(2) | 77.25(6) |
| O(1)$^{i}$-Co(1)-N(3)$^{iii}$ | 90.99(6) | N(1)$^{i}$-Co(1)-N(1) | 180.000(1) | O(5)$^{iv}$-Co(2)-N(2) | 85.80(6) |
| N(3)$^{ii}$-Co(1)-N(3)$^{iii}$ | 180.000(1) | O(4)$^{iv}$-Co(2)-O(4) | 180.000(1) | O(5)-Co(2)-N(2) | 94.20(6) |
| O(1)-Co(1)-N(1)$^{i}$ | 101.92(6) | O(4)$^{iv}$-Co(2)-O(5)$^{iv}$ | 90.67(6) | O(4)-Co(2)-N(2)$^{iv}$ | 102.75(6) |
| N(3)$^{ii}$-Co(1)-N(1)$^{i}$ | 86.74(6) | O(4)-Co(2)-O(5)$^{iv}$ | 89.33(6) | N(2)-Co(2)-N(2)$^{iv}$ | 180.00(8) |
| | | | Complex **4** | | |
| Zn(1)-O(3)$^{i}$ | 1.9579(17) | Zn(1)-O(5) | 2.0638(18) | Zn(2)-N(1) | 2.2574(18) |
| Zn(1)-O(1) | 2.0204(17) | Zn(1)-N(3)$^{ii}$ | 2.0916(18) | | |
| O(3)$^{i}$-Zn(1)-O(1) | 171.75(7) | O(1)-Zn(1)-N(3)$^{ii}$ | 95.24(7) | O(1)-Zn(1)-N(1) | 76.59(6) |
| O(3)$^{i}$-Zn(1)-O(5) | 94.49(7) | O(5)-Zn(1)-N(3)$^{ii}$ | 105.59(7) | O(5)-Zn(1)-N(1) | 133.61(6) |
| O(1)-Zn(1)-O(5) | 87.29(7) | O(3)$^{i}$-Zn(1)-N(1) | 96.49(7) | N(3)$^{ii}$-Zn(1)-N(1) | 118.84(7) |
| O(3)$^{i}$-Zn(1)-N(3)$^{ii}$ | 92.04(7) | | | | |
| | | | Complex **5** | | |
| Cd(1)-O(2)$^{i}$ | 2.254(2) | Cd(1)-O(1)$^{iii}$ | 2.279(2) | Cd(1)-O(4) | 2.430(2) |
| Cd(1)-N(4)$^{ii}$ | 2.267(2) | Cd(1)-O(3) | 2.395(2) | Cd(1)-O(3)$^{iv}$ | 2.576(2) |
| Cd(1)-O(4)$^{v}$ | 2.649(2) | | | | |
| O(2)$^{i}$-Cd(1)-N(4)$^{ii}$ | 94.24(8) | N(4)$^{ii}$-Cd(1)-O(4) | 150.27(9) | O(4)-Cd(1)-O(3)$^{iv}$ | 71.94(7) |
| O(2)$^{i}$-Cd(1)-O(1)$^{iii}$ | 173.18(10) | O(1)$^{iii}$-Cd(1)-O(4) | 85.64(8) | O(2)$^{i}$-Cd(1)-O(4)$^{v}$ | 95.82(8) |
| N(4)$^{ii}$-Cd(1)-O(1)$^{iii}$ | 86.08(9) | O(3)-Cd(1)-O(4) | 55.06(8) | N(4)$^{ii}$-Cd(1)-O(4)$^{v}$ | 83.04(9) |

| | | | | | |
|---|---|---|---|---|---|
| $O(2)^{i}$-Cd(1)-O(3) | 84.47(8) | $O(2)^{i}$-Cd(1)-$O(3)^{iv}$ | 79.24(8) | $O(1)^{iii}$-Cd(1)-$O(4)^{v}$ | 77.45(8) |
| $N(4)^{ii}$-Cd(1)-O(3) | 153.86(9) | $N(4)^{ii}$-Cd(1)-$O(3)^{iv}$ | 83.50(9) | O(3)-Cd(1)-$O(4)^{v}$ | 71.17(7) |
| $O(1)^{iii}$-Cd(1)-O(3) | 92.23(8) | $O(1)^{iii}$-Cd(1)-$O(3)^{iv}$ | 107.55(8) | O(4)-Cd(1)-$O(4)^{v}$ | 122.67(7) |
| $O(2)^{i}$-Cd(1)-O(4) | 97.27(8) | O(3)-Cd(1)-$O(3)^{iv}$ | 121.60(7) | $O(3)^{iv}$-Cd(1)-$O(4)^{v}$ | 165.27(7) |

[a] Symmetry transformations used to generate equivalent atoms for **1**: i) -x+3/2, y-1/2, -z+1/2. For **2**: x+1/2, -y+1/2, z-1/2. For **3**: i) -x+1, -y+1, -z+2. ii) -x+2, -y+1, -z+2. iii) x-1, y, z. iv) -x+2, -y+2, -z+1. For 4: i) -x, y+1/2, -z+1/2. ii) -x, -y, -z. For **5**: i) -x+1, y+1/2, -z+1/2. ii) x, y+1, z. iii) -x+3/2, -y+1, z+1/2. iv) x-1/2, -y+3/2, -z+1. v) x+1/2, -y+3/2, -z+1.

**Table S2** Geometrical Parameters of Hydrogen Bonds (Å, °) for complexes **1-5**

| D-H···A | d(D-H) ( Å) | d(H···A) ( Å) | d(D···A) ( Å) | **<(DHA)** | Symmetry codes |
|---|---|---|---|---|---|
| | | | Complex **1** | | |
| O5-H1w··O3 | 0.85 | 1.82 | 2.666(3) | 173.8 | x-1/2, -y+1/2, z+1/2 |
| O5-H2w···O2 | 0.85 | 1.88 | 2.710(3) | 167.1 | -x+2, -y, -z+1 |
| O6-H3w··O2 | 0.85 | 1.96 | 2.811(3) | 175.1 | -x+2, -y+1, -z+1 |
| O6-H4w···N3 | 0.85 | 1.95 | 2.768(3) | 162.5 | -x+1, -y+1, -z+1 |
| | | | Complex **2** | | |
| O5-H1w···O2 | 0.85 | 1.77 | 2.609(2) | 170.8 | -x+5/2, y+1/2, -z+3/2 |
| O5-H2w···O3 | 0.85 | 1.97 | 2.767(2) | 156.4 | -x+2, -y, -z+2 |
| O6-H3w···N3 | 0.85 | 1.86 | 2.705(3) | 170.9 | -x+3/2, y-1/2, -z+3/2 |
| O6-H4w···O3 | 0.85 | 1.96 | 2.746(2) | 153.3 | -x+3/2, y+1/2, -z+3/2 |
| | | | Complex **3** | | |
| O5-H1w···O3 | 0.85 | 1.80 | 2.644(2) | 175.2 | -x+1, -y+2, -z+1 |
| O5-H2w···O2 | 0.85 | 1.85 | 2.697(2) | 173.4 | x+1, y, z-1 |
| | | | Complex **4** | | |
| O5-H2w···O3 | 0.85 | 2.63 | 3.268(2) | 132.5 | x, -y+1/2, z-1/2 |
| O5-H2w···O4 | 0.85 | 1.89 | 2.724(2) | 167.6 | x, -y+1/2, z-1/2 |
| O5-H1w···O2 | 0.85 | 1.88 | 2.697(2) | 162.0 | -x+1, y+1/2, -z+1/2 |