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# Synthesis, structures and photoluminescence of a new series of 3D coordination polymers constructed from 2,2'-bipyridine-3,3'-dicarboxylic acid 1,1'-dioxide and oxalic acid

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**Chart S1** The ligands' structural formulae and abbreviations used in the present work

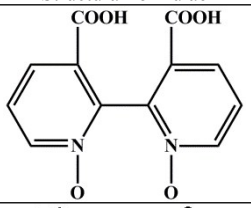
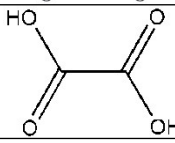
| Name of ligands | Structural formulae | Abbreviations |
|---|---|---|
| 2,2'-bipyridine-3,3'-dicarboxylic acid 1,1'-dioxide, |  | $H_2$bdcd |
| oxalic aid |  | $H_2$ox |

**Table S1.** Selected bond lengths [Å] and angles [deg] for compound **2**.

| Bond | Distance | Bond | Distance |
|---|---|---|---|
| Tb(1)-O(6) | 2.272(4) | Tb(1)-O(7)#2 | 2.403(4) |
| Tb(1)-O(14) | 2.373(4) | Tb(1)-O(5)#1 | 2.390(4) |
| Tb(1)-O(13) | 2.397(4) | Tb(1)-O(15W) | 2.399(4) |
| Tb(1)-O(8) | 2.365(3) | Tb(1)-O(16W) | 2.434(4) |
| Tb(2)-O(4)#3 | 2.362(4) | Tb(2)-O(17W) | 2.378(4) |
| Tb(2)-O(10) | 2.415(4) | Tb(2)-O(2)#4 | 2.393(4) |
| Tb(2)-O(11) | 2.503(4) | Tb(2)-O(9)#5 | 2.436(4) |
| Tb(2)-O(12) | 2.389(4) | Tb(2)-O(1)#4 | 2.508(4) |
| Tb(2)-O(3)#3 | 2.599(4) | | |

| Moiety | Angle | Moiety | Angle |
|---|---|---|---|
| O(6)-Tb(1)-O(8) | 143.67(15) | O(12)-Tb(2)-O(10) | 137.73(13) |
| O(14)-Tb(1)-O(8) | 112.31(13) | O(4)#3-Tb(2)-O(9)#5 | 135.79(12) |
| O(6)-Tb(1)-O(14) | 82.69(13) | O(17W)-Tb(2)-O(9)#5 | 75.88(15) |
| O(6) -Tb(1)-O(5)#1 | 110.19(13) | O(2)#4-Tb(2)-O(9)#5 | 68.67(12) |
| O(8)-Tb(1)-O(5)#1 | 73.62(12) | O(12)-Tb(2)-O(9)#5 | 113.18(14) |
| O(14)-Tb(1)-O(5)#1 | 150.20(15) | O(10)-Tb(2)-O(9)#5 | 66.93(12) |
| O(6)-Tb(1)-O(13) | 140.26(14) | O(4)#3-Tb(2)-O(11) | 74.89(13) |
| O(8)-Tb(1)-O(13) | 74.80(14) | O(17W)-Tb(2)-O(11) | 144.83(15) |
| O(14)-Tb(1)-O(13) | 68.29(13) | O(2)#4-Tb(2)-O(11) | 102.28(13) |
| O(5)#1-Tb(1)-O(13) | 86.43(13) | O(12)-Tb(2)-O(11) | 65.78(13) |
| O(6)-Tb(1)-O(15W) | 74.57(14) | O(10)-Tb(2)-O(11) | 75.65(13) |
| O(8)-Tb(1)-O(15W) | 138.74(15) | O(9)#5-Tb(2)-O(11) | 71.09(14) |
| O(14) -Tb(1)-O(15W) | 80.02(15) | O(4)#3-Tb(2)-O(1)#4 | 84.72(13) |
| O(5)#1-Tb(1)-O(15W) | 77.99(15) | O(17W)-Tb(2)-O(1)#4 | 82.69(15) |
| O(15w)-Tb(1)-O(13) | 74.13(14) | O(2)#4-Tb(2)-O(1)#4 | 72.84(12) |
| O(6)-Tb(1)-O()#2 | 78.09(13) | O(12)-Tb(2)-O(1)#4 | 66.31(13) |
| O(8)-Tb(1)-O(7)#2 | 68.79(13) | O(10)-Tb(2)-O(1)#4 | 142.64(13) |
| O(14)-Tb(1)-O(7)#2 | 138.05(14) | O(9)#5-Tb(2)-O(1)#4 | 139.32(12) |
| O(5)#1-Tb(1)-O(7)#2 | 71.74(14) | O(11)-Tb(2)-O(1)#4 | 131.10(14) |
| O(13)-Tb(1)-O(7)#2 | 141.44(12) | O(4)#3-Tb(2)-O(3)#3 | 52.56(14) |
| O(15W)-Tb(1)-O(7)#2 | 128.48(14) | O(17W)-Tb(2)-O(3)#3 | 72.69(14) |
| O(6)-Tb(1)-O(16W) | 79.61(13) | O(2)#4-Tb(2)-O(3)#3 | 134.51(12) |
| O(8)-Tb(1)-O(16W) | 74.83(14) | O(12)-Tb(2)-O(3)#3 | 114.62(14) |
| O(14)-Tb(1)-O(16W) | 71.50(15) | O(10)-Tb(2)-O(3)#3 | 72.01(13) |
| O(5)#1-Tb(1)-O(16W) | 135.93(15) | O(9)#5-Tb(2)-O(3)#3 | 131.33(14) |
| O(13)-Tb(1)-O(16W) | 113.81(14) | O(11)-Tb(2)-O(3)#3 | 122.27(12) |
| O(15W)-Tb(1)-O(16W) | 143.57(15) | O(1)#4-Tb(2)-O(3)#3 | 71.17(12) |
| O(7)#2-Tb(1)-O(16W) | 68.56(14) | O(4)#3-Tb(2)-C(6)#3 | 26.10(16) |
| O(17w)-Tb(2)-O(4)#3 | 124.96(14) | O(17W)-Tb(2)-C(6)#3 | 98.94(16) |
| O(4)#3-Tb(2)-O(2)#4 | 147.45(15) | O(2)#4-Tb(2)-C(6)#3 | 150.40(14) |
| O(17W)-Tb(2)-O(2)#4 | 76.01(14) | O(12)-Tb(2)-C(6)#3 | 96.03(16) |
| O(4)#3-Tb(2)-O(12) | 75.91(14) | O(10)-Tb(2)-C(6)#3 | 72.32(15) |
| O(17W)-Tb(2)-O(12) | 141.59(13) | O(9)#5-Tb(2)-C(6)#3 | 139.24(14) |
| O(12)-Tb(2)-O(2)#4 | 73.61(14) | O(11)-Tb(2)-C(6)#3 | 98.18(15) |
| O(4)#3-Tb(2)-O(10) | 78.01(14) | O(1)#4-Tb(2)-C(6)#3 | 77.61(14) |
| O(17W)-Tb(2)-O(10) | 80.65(14) | O(3)#3-Tb(2)-C(6)#3 | 26.50(15) |
| O(2)#4-Tb(2)-O(10) | 133.53(14) | | |

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1,-*y*+1,-*z*； #2 -*x*+1,-*y*+1,-*z*； #3 –*x*+*1*,-*y*,-*z*； #4 –*x*+2,-*y*,-*z*； #5 -*x*+1,-*y*,-*z*+1

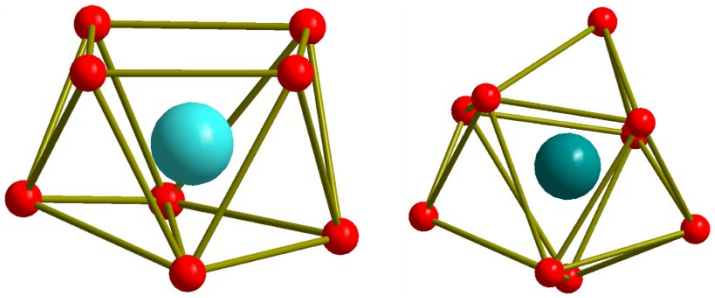



**Figure S1** The coordination geometry of Eu1 (a) and Eu2 (b) in compound **1**.

**Table S2** Selected intermolecular hydrogen bond for compound **1**

| Donor-H…Acceptor | [ARU ] | D-H (Å) | H…A (Å) | D…A (Å) | D-H…A (°) |
|---|---|---|---|---|---|
| O(15W)-H(15A)…O(18W) | [ ] | 0.85 | 1.99 | 2.821 | 169 |
| O(15W)-H(15B)…O(7) | [1655] | 0.85 | 1.95 | 2.735 | 154 |
| O(16W)-H(16B) ..O(1) | [1455] | 0.86 | 2.11 | 2.934 | 163 |
| O(16W)-H(16A)…O(12) | [2655] | 0.85 | 2.16 | 2.771 | 128 |
| O(16W)-H(16A)…O(14) | [2655] | 0.86 | 2.55 | 3.392 | 170 |
| O(17W)-H(17A)…O(19W) | [2655] | 0.85 | 1.89 | 2.707 | 161 |
| O(17W)-H(17B)…O(21W) | [2755] | 0.85 | 1.94 | 2.766 | 165 |
| O(18W)-H(18A)…O(9) | [2656] | 0.85 | 2.35 | 3.058 | 141 |
| O(18W)-H(18B)…O(20W) | [2755] | 0.85 | 2.13 | 2.946 | 160 |
| O(19W)-H(19A)…O(3) | [ ] | 0.85 | 2.08 | 2.760 | 137 |
| O(19W)-H(19B)…O(21W) | [2664] | 0.85 | 2.04 | 2.861 | 162 |
| O(20W)-H(20A)…O(11) | [2655] | 0.85 | 2.08 | 2.885 | 159 |
| O(20W)-H(20B)…O(2) | [ ] | 0.85 | 1.99 | 2.768 | 151 |
| O(21W)-H(21A)…O(20W) | [2754] | 0.85 | 1.89 | 2.740 | 172 |
| O(21W)-H(21B)…O(10) | [2655] | 0.85 | 2.00 | 2.842 | 170 |

Translation of ARU-code to equivalent position code: [2655] = 1-*x*,-*y*,-*z*; [2656] = 1-*x*,-*y*,1-*z*; [1655] = 1+*x*,*y*,*z*; [2755] = 2-*x*,-*y*,-*z*; [1455] = -1+*x*,*y*,*z*; [2664] = 1-*x*,1-*y*,-1-*z*; [2765] = 2-*x*,1-*y*,-*z*; [1565] = *x*,1+*y*,*z*; [2754] = 2-*x*,-*y*,-1-*z*.

**Table S3** Selected intermolecular hydrogen bond for compound **2**

| Donor-H…Acceptor | [ARU ] | D-H (Å) | H…A (Å) | D…A (Å) | D-H…A (°) |
|---|---|---|---|---|---|
| O(15W)--H(15A)...O(18W) | [ ] | 0.85 | 1.98 | 2.808 | 164 |
| O(15W)--H(15B)...O(7) | [1655] | 0.84 | 1.93 | 2.749 | 165 |
| O(16W)--H(16A)...O(12) | [2655] | 0.85 | 2.19 | 2.757 | 125 |
| O(16W)--H(16A)...O(14) | [2655] | 0.85 | 2.53 | 3.371 | 177 |
| O(16W)--H(16B)...O(1) | [1455] | 0.85 | 2.11 | 2.924 | 159 |
| O(17W)--H(17A)...O(19W) | [2655] | 0.85 | 1.87 | 2.707 | 166 |
| O(17W)--H(17B)...O(21W) | [2755] | 0.85 | 1.90 | 2.748 | 173 |
| O(18W)--H(18A)...O(9) | [2656] | 0.85 | 2.32 | 3.040 | 144 |
| O(18W)--H(18B)...O(20W) | [2755] | 0.85 | 2.17 | 2.940 | 151 |
| O(19W)--H(19A)...O(3) | [ ] | 0.85 | 2.04 | 2.753 | 140 |
| O(19W)--H(19B)...O(21W) | [2664] | 0.85 | 2.02 | 2.848 | 166 |
| O(20W)--H(20A)...O(11) | [2655] | 0.85 | 2.08 | 2.869 | 154 |
| O(20W)--H(20B)...O(2) | [ ] | 0.85 | 1.94 | 2.771 | 167 |
| O(20W)--H(20B)...N(2) | [ ] | 0.85 | 2.61 | 3.291 | 138 |
| O(21W)--H(21A)...O(20W) | [2754] | 0.85 | 1.95 | 2.743 | 156 |
| O(21W)--H(21B)...O(3) | [2655] | 0.85 | 2.00 | 2.841 | 173 |

Translation of ARU-code to equivalent position code: [2655] = 1-x,-y,-z; [2656] = 1-x,-y,1-z; [1655] = 1+x,y,z; [2755] = 2-x,-y,-z; [1455] = -1+x,y,z; [2765] = 2-x,1-y,-z; [2664] = 1-x,1-y,-1-z; [1565] = x,1+y,z; [2754] = 2-x,-y,-1-z.

The total potential solvent volume is 236.4 Å$^3$ accounting for *ca*. 19.4% of per cell volume 1216.7 Å$^3$ calculated by the Platon program for the compound **2** .[A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*, Utrecht University Press, The Netherlands, 2006.]

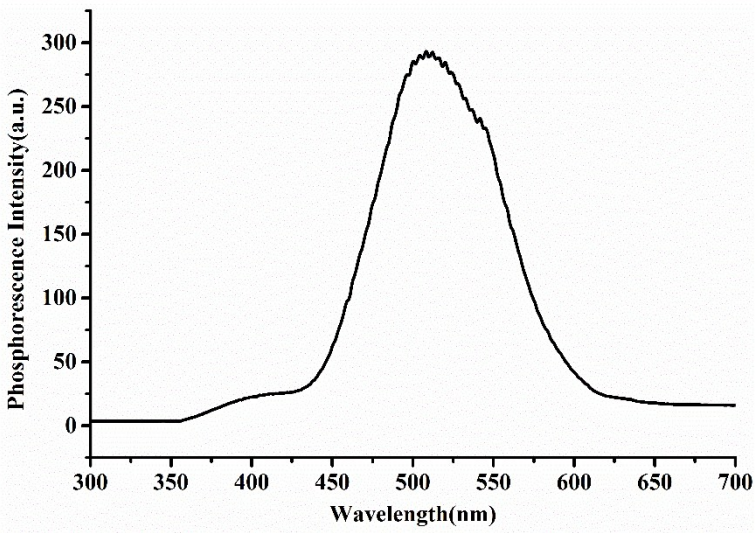



**Figure S2** The phosphorescence spectrum of compound **5** at 77K

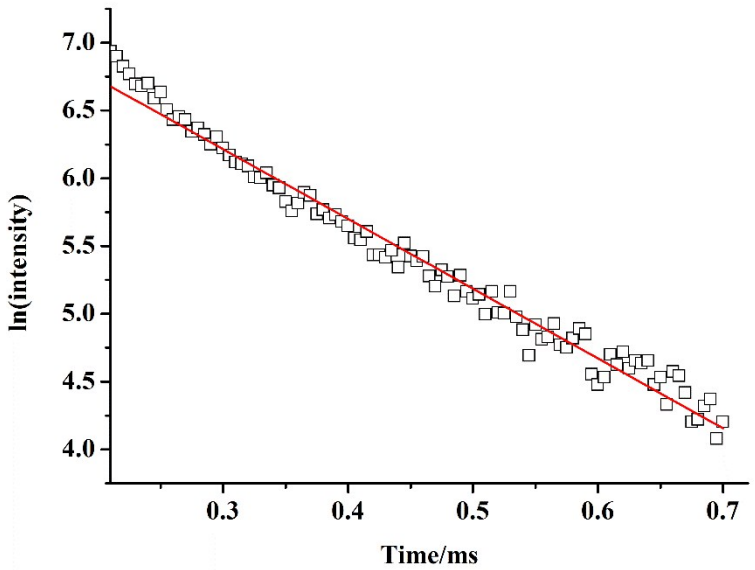



**Figure S3** Room temperature emission decay curve of compound **1** excited at 280 nm and monitored at 615 nm.