

Supporting Information for

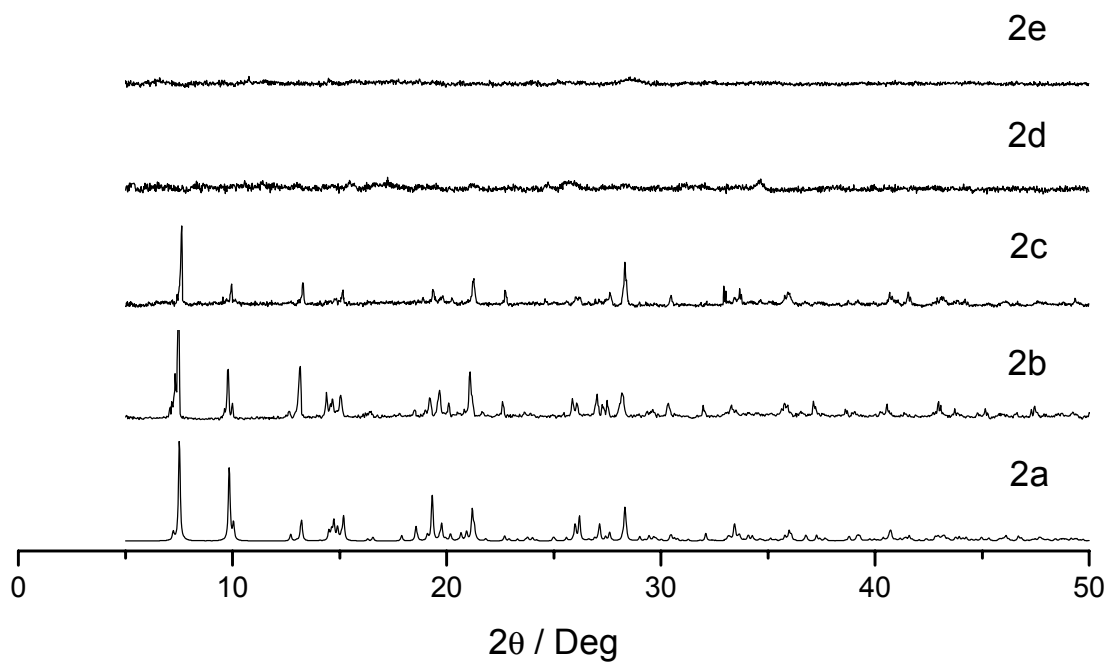
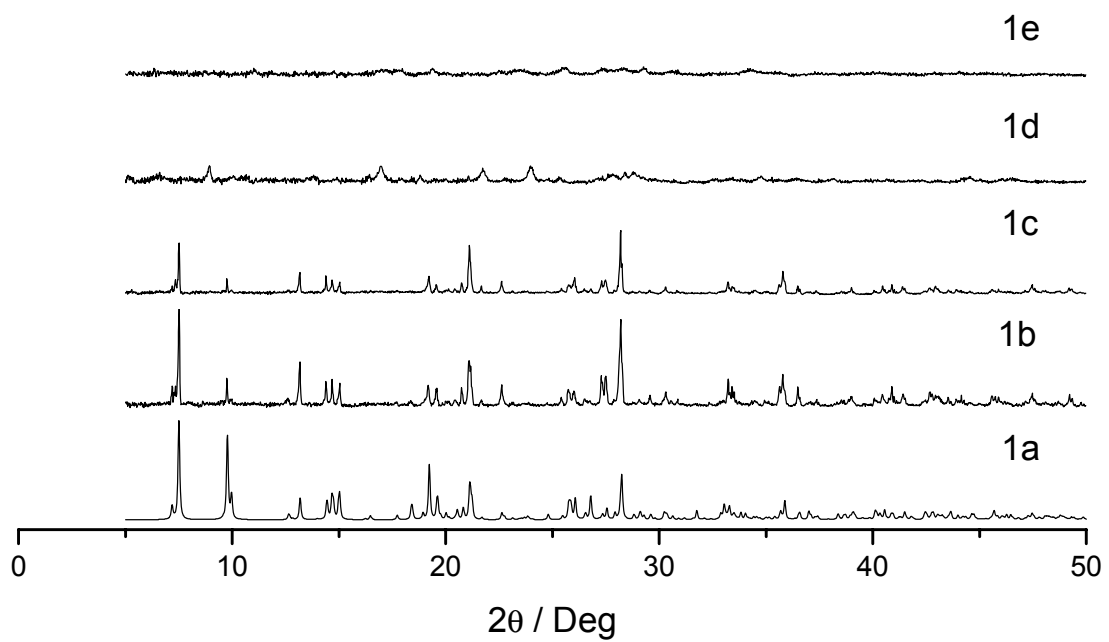
Unprecedented Na^I-Cu^{II}-Ln^{III} heterometallic coordination polymers based on 3,5-pyrazoledicarboxylate with both infinite cationic and anionic chains

Yan Wang,^{a,b} You Song,^a Zhao-Rui Pan,^a Ying-Zhong Shen,^b Zheng Hu,^a Zi-Jian Guo,^a and He-Gen Zheng^{*a}

^a State Key Laboratory of Coordination Chemistry and Key Laboratory for Mesoscopic Chemistry of Ministry of Education College of Chemistry and Chemical Engineering, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, P. R. China. E-mail: zhenghg@nju.edu.cn; Fax: 86-25-83314502; Tel: 86-25-83686155

^b Applied Chemistry Department, School of Material Science & Engineering, Nanjing University of Aeronautics & Astronautics, Nanjing 210016, P. R. China

***Corresponding author: Prof. Zheng E-mail: zhenghg@nju.edu.cn; Fax: 86-25-83314502; Tel: 86-25-83686155**



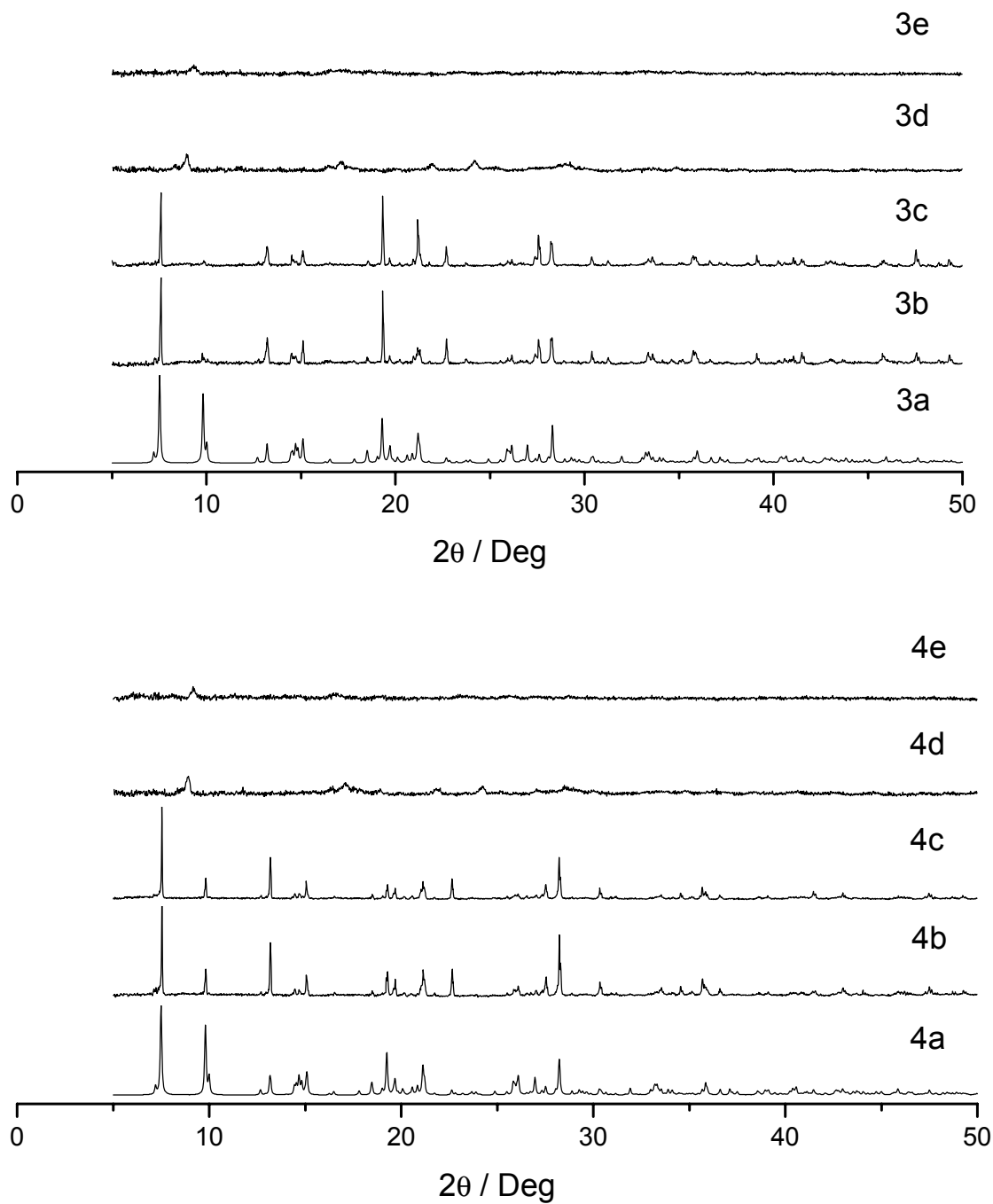


Fig. S1 Simulated and experimental XRPD patterns of complexes 1–4: the simulated (a); the experimental at 25°C (b), 60°C (c), 150°C (d) and 220°C (e).

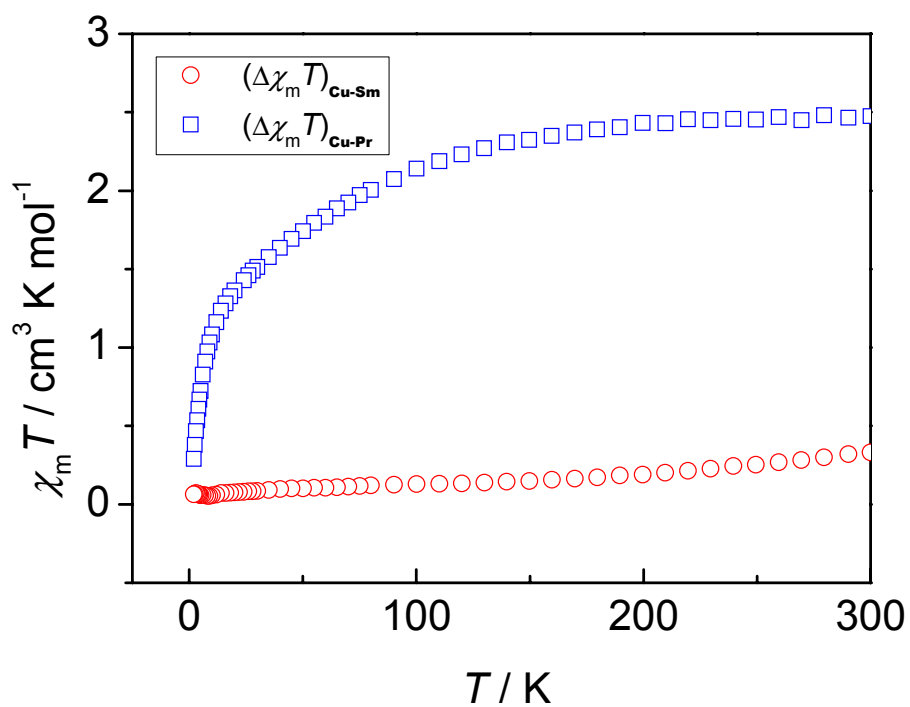


Fig. S2 Thermal dependence of $(\Delta\chi_m T)_{\text{Cu-Ln}}$: $(\Delta\chi_m T)_{\text{Cu-Sm}} = (\chi_m T)_{\text{Cu-Sm}} - (\chi_m T)_{\text{Cu-La}}$ and $(\Delta\chi_m T)_{\text{Cu-Pr}} = (\chi_m T)_{\text{Cu-Pr}} - (\chi_m T)_{\text{Cu-La}}$

Table S1. Selected bond lengths (Å) and bond angles (°) for 1–4

| Complex 1 | | | | | |
|--|----------|---------------------------|----------|---------------------------|----------|
| Na1—O14 | 2.353(4) | Cu1—N3 | 1.920(3) | La1—O10 | 2.583(3) |
| Na1—O15 | 2.403(4) | Cu1—O1 | 2.001(3) | La1—O11 | 2.584(3) |
| Na1—O15 ⁱ | 2.412(4) | Cu1—O5 | 1.975(3) | La1—O12 | 2.487(3) |
| Na1—O14 ⁱⁱ | 2.418(4) | Cu1—O9 | 2.344(3) | La1—O13 | 2.581(3) |
| Na1—O16 | 2.454(4) | La1—O3 | 2.612(3) | La1—N2 | 2.649(3) |
| Na1—O17 | 2.584(6) | La1—O4 ⁱⁱⁱ | 2.595(3) | La1—N4 | 2.615(3) |
| Cu1—N1 | 1.928(3) | La1—O7 | 2.553(3) | | |
| O14—Na1—O15 | 104.8(1) | O5—Cu1—O9 | 94.3(1) | O13—La1—O3 | 71.6(1) |
| O15—Na1—O15 ⁱ | 85.3(1) | O1—Cu1—O9 | 94.8(1) | O10—La1—O3 | 97.0(1) |
| O14—Na1—O14 ⁱⁱ | 86.3(1) | O12—La1—O7 | 69.8(1) | O11—La1—O3 | 69.6(1) |
| O15 ⁱ —Na1—O14 ⁱⁱ | 83.6(1) | O12—La1—O13 | 75.7(1) | O4 ⁱⁱⁱ —La1—O3 | 143.0(1) |
| O14—Na1—O16 | 89.7(1) | O7—La1—O13 | 70.0(1) | O12—La1—N4 | 130.5(1) |
| O15—Na1—O16 | 91.5(1) | O12—La1—O10 | 138.9(1) | O7—La1—N4 | 61.6(1) |
| O15 ⁱ —Na1—O16 | 89.6(1) | O7—La1—O10 | 127.4(1) | O13—La1—N4 | 79.6(1) |
| O14 ⁱⁱ —Na1—O16 | 88.0(1) | O13—La1—O10 | 142.4(1) | O10—La1—N4 | 82.4(1) |
| O14—Na1—O17 | 82.8(2) | O12—La1—O11 | 72.0(1) | O11—La1—N4 | 147.2(1) |
| O15—Na1—O17 | 71.8(2) | O7—La1—O11 | 126.0(1) | O4 ⁱⁱⁱ —La1—N4 | 84.0(1) |
| O15 ⁱ —Na1—O17 | 101.1(2) | O13—La1—O11 | 133.0(1) | O3—La1—N4 | 131.1(1) |
| O14 ⁱⁱ —Na1—O17 | 110.9(2) | O10—La1—O11 | 68.5(1) | O12—La1—N2 | 137.0(1) |
| O16—Na1—O17 | 159.1(2) | O12—La1—O4 ⁱⁱⁱ | 85.2(1) | O7—La1—N2 | 127.0(1) |
| N1—Cu1—O1 | 82.2(1) | O7—La1—O4 ⁱⁱⁱ | 66.5(1) | O13—La1—N2 | 75.6(1) |
| N3—Cu1—O5 | 82.4(1) | O13—La1—O4 ⁱⁱⁱ | 136.2(1) | O10—La1—N2 | 67.8(1) |
| N3—Cu1—N1 | 98.3(1) | O10—La1—O4 ⁱⁱⁱ | 73.3(1) | O11—La1—N2 | 107.0(1) |
| O5—Cu1—O1 | 96.0(1) | O11—La1—O4 ⁱⁱⁱ | 73.7(1) | O4 ⁱⁱⁱ —La1—N2 | 137.0(1) |
| N3—Cu1—O9 | 91.6(1) | O12—La1—O3 | 79.4(1) | O3—La1—N2 | 61.5(1) |
| N1—Cu1—O9 | 94.5(1) | O7—La1—O3 | 135.3(1) | N4—La1—N2 | 73.6(1) |
| Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $-x+1, -y, -z+1$; (iii) $x, -y+1, z+1/2$. | | | | | |
| Complex 2 | | | | | |
| Na1—O14 | 2.410(4) | Cu1—N3 | 1.916(3) | Sm1—O10 | 2.477(3) |
| Na1—O14 ⁱ | 2.377(4) | Cu1—O1 | 1.993(2) | Sm1—O11 | 2.496(3) |
| Na1—O15 | 2.336(4) | Cu1—O5 | 1.972(3) | Sm1—O12 | 2.395(3) |
| Na1—O15 ⁱⁱ | 2.391(3) | Cu1—O9 | 2.327(3) | Sm1—O13 | 2.476(3) |
| Na1—O16 | 2.451(4) | Sm1—O3 | 2.550(3) | Sm1—N2 | 2.571(3) |
| Na1—O17 | 2.626(6) | Sm1—O4 ⁱⁱⁱ | 2.569(3) | Sm1—N4 | 2.530(3) |
| Cu1—N1 | 1.918(3) | Sm1—O7 | 2.487(3) | | |
| O15—Na1—O14 ⁱ | 102.4(1) | N1—Cu1—O9 | 93.9(1) | O10—Sm1—O3 | 96.4(1) |
| O15—Na1—O15 ⁱⁱ | 87.4(1) | O5—Cu1—O9 | 95.9(1) | O7—Sm1—O3 | 134.4(1) |
| O14 ⁱ —Na1—O15 ⁱⁱ | 170.2(1) | O1—Cu1—O9 | 94.6(1) | O11—Sm1—O3 | 69.3(1) |
| O15—Na1—O14 | 171.6(1) | O12—Sm1—O13 | 76.2(1) | N4—Sm1—O3 | 134.0(1) |
| O14 ⁱ —Na1—O14 | 86.1(1) | O12—Sm1—O10 | 138.4(1) | O12—Sm1—O4 ⁱⁱⁱ | 84.5(1) |
| O15 ⁱⁱ —Na1—O14 | 84.2(1) | O13—Sm1—O10 | 142.0(1) | O13—Sm1—O4 ⁱⁱⁱ | 135.9(1) |
| O15—Na1—O16 | 90.6(1) | O12—Sm1—O7 | 68.6(1) | O10—Sm1—O4 ⁱⁱⁱ | 74.5(1) |

| | | | | | |
|----------------------------|----------|-------------|----------|---------------------------|----------|
| O14 ⁱ —Na1—O16 | 91.7(1) | O13—Sm1—O7 | 70.1(1) | O7—Sm1—O4 ⁱⁱⁱ | 66.0(1) |
| O15 ⁱⁱ —Na1—O16 | 86.8(1) | O10—Sm1—O7 | 129.2(1) | O11—Sm1—O4 ⁱⁱⁱ | 71.8(1) |
| O14—Na1—O16 | 89.0(1) | O12—Sm1—O11 | 71.2(1) | N4—Sm1—O4 ⁱⁱⁱ | 83.6(1) |
| O15—Na1—O17 | 81.2(2) | O13—Sm1—O11 | 134.2(1) | O3—Sm1—O4 ⁱⁱⁱ | 140.6(1) |
| O14 ⁱ —Na1—O17 | 71.2(2) | O10—Sm1—O11 | 68.2(1) | O12—Sm1—N2 | 136.2(1) |
| O15 ⁱⁱ —Na1—O17 | 112.1(2) | O7—Sm1—O11 | 123.2(1) | O13—Sm1—N2 | 75.5(1) |
| O14—Na1—O17 | 101.9(2) | O12—Sm1—N4 | 131.5(1) | O10—Sm1—N2 | 67.4(1) |
| O16—Na1—O17 | 158.8(2) | O13—Sm1—N4 | 80.6(1) | O7—Sm1—N2 | 129.1(1) |
| N3—Cu1—N1 | 97.2(1) | O10—Sm1—N4 | 82.0(1) | O11—Sm1—N2 | 107.7(1) |
| N3—Cu1—O5 | 82.7(1) | O7—Sm1—N4 | 63.5(1) | N4—Sm1—N2 | 74.9(1) |
| N1—Cu1—O1 | 82.7(1) | O11—Sm1—N4 | 145.2(1) | O3—Sm1—N2 | 62.7(1) |
| O5—Cu1—O1 | 96.3(1) | O12—Sm1—O3 | 77.5(1) | O4 ⁱⁱⁱ —Sm1—N2 | 138.2(1) |
| N3—Cu1—O9 | 92.1(1) | O13—Sm1—O3 | 72.9(1) | | |

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $-x+1, -y+1, -z+2$; (iii) $x, -y+1, z-1/2$.

Complex 3

| | | | | | |
|---|----------|-----------------------|----------|---------------------------|----------|
| Na1—O14 | 2.333(5) | Cu1—N3 | 1.922(4) | Pr1—O10 | 2.537(3) |
| Na1—O14 ⁱⁱ | 2.409(4) | Cu1—O1 | 1.994(3) | Pr1—O11 | 2.540(4) |
| Na1—O15 | 2.400(5) | Cu1—O5 | 1.969(4) | Pr1—O12 | 2.433(3) |
| Na1—O15 ⁱ | 2.395(4) | Cu1—O9 | 2.337(3) | Pr1—O13 | 2.521(3) |
| Na1—O16 | 2.453(4) | Pr1—O3 | 2.575(4) | Pr1—N2 | 2.606(4) |
| Na1—O17 | 2.623(8) | Pr1—O4 ⁱⁱⁱ | 2.578(3) | Pr1—N4 | 2.567(4) |
| Cu1—N1 | 1.925(4) | Pr1—O7 | 2.511(3) | | |
| O14—Na1—O15 ⁱ | 103.5(2) | N1—Cu1—O9 | 94.3(2) | O13—Pr1—O3 | 72.0(1) |
| O14—Na1—O15 | 170.7(2) | O5—Cu1—O9 | 95.0(1) | O10—Pr1—O3 | 96.2(1) |
| O15 ⁱ —Na1—O15 | 85.8(2) | O1—Cu1—O9 | 94.6(1) | O11—Pr1—O3 | 69.5(1) |
| O14—Na1—O14 ⁱⁱ | 86.7(1) | O12—Pr1—O7 | 69.4(1) | N4—Pr1—O3 | 132.4(1) |
| O15 ⁱ —Na1—O14 ⁱⁱ | 169.8(2) | O12—Pr1—O13 | 75.7(1) | O12—Pr1—O4 ⁱⁱⁱ | 85.0(1) |
| O15—Na1—O14 ⁱⁱ | 84.0(2) | O7—Pr1—O13 | 70.1(1) | O7—Pr1—O4 ⁱⁱⁱ | 66.4(1) |
| O14—Na1—O16 | 90.5(2) | O12—Pr1—O10 | 138.7(1) | O13—Pr1—O4 ⁱⁱⁱ | 136.3(1) |
| O15 ⁱ —Na1—O16 | 91.8(2) | O7—Pr1—O10 | 128.8(1) | O10—Pr1—O4 ⁱⁱⁱ | 74.3(1) |
| O15—Na1—O16 | 89.1(2) | O13—Pr1—O10 | 141.9(1) | O11—Pr1—O4 ⁱⁱⁱ | 72.8(1) |
| O14 ⁱⁱ —Na1—O16 | 87.1(1) | O12—Pr1—O11 | 72.0(1) | N4—Pr1—O4 ⁱⁱⁱ | 83.9(1) |
| O14—Na1—O17 | 81.6(2) | O7—Pr1—O11 | 125.0(1) | O3—Pr1—O4 ⁱⁱⁱ | 141.8(1) |
| O15 ⁱ —Na1—O17 | 70.8(2) | O13—Pr1—O11 | 133.5(1) | O12—Pr1—N2 | 136.3(1) |
| O15—Na1—O17 | 102.0(2) | O10—Pr1—O11 | 67.9(1) | O7—Pr1—N2 | 127.9(1) |
| O14 ⁱⁱ —Na1—O17 | 112.1(2) | O12—Pr1—N4 | 131.0(1) | O13—Pr1—N2 | 75.4(1) |
| O16—Na1—O17 | 158.5(2) | O7—Pr1—N4 | 62.5(1) | O10—Pr1—N2 | 67.4(1) |
| N3—Cu1—N1 | 97.8(2) | O13—Pr1—N4 | 80.0(1) | O11—Pr1—N2 | 107.1(1) |
| N3—Cu1—O5 | 82.5(2) | O10—Pr1—N4 | 82.5(1) | N4—Pr1—N2 | 74.2(1) |
| N1—Cu1—O1 | 82.4(2) | O11—Pr1—N4 | 146.2(1) | O3—Pr1—N2 | 61.9(1) |
| O5—Cu1—O1 | 96.3(1) | O12—Pr1—O3 | 78.3(1) | O4 ⁱⁱⁱ —Pr1—N2 | 137.7(1) |
| N3—Cu1—O9 | 91.8(1) | O7—Pr1—O3 | 134.9(1) | | |

Symmetry codes: (i) $-x+1, y, -z+1/2$; (ii) $-x+1, -y+1, -z$; (iii) $x, -y, z+1/2$.

Complex 4

| | | | | | |
|-----------------------|----------|-----------------------|----------|---------|----------|
| Na1—O14 | 2.416(3) | Cu1—N4 | 1.924(3) | Nd1—O10 | 2.526(3) |
| Na1—O14 ⁱ | 2.346(4) | Cu1—O1 | 1.979(3) | Nd1—O11 | 2.527(3) |
| Na1—O15 ⁱⁱ | 2.400(4) | Cu1—O5 | 1.997(3) | Nd1—O12 | 2.430(3) |
| Na1—O15 | 2.413(4) | Cu1—O9 | 2.339(3) | Nd1—O13 | 2.509(3) |
| Na1—O16 | 2.460(4) | Nd1—O3 | 2.514(3) | Nd1—N1 | 2.567(3) |
| Na1—O17 | 2.620(6) | Nd1—O7 | 2.570(3) | Nd1—N3 | 2.602(3) |
| Cu1—N2 | 1.918(3) | Nd1—O8 ⁱⁱⁱ | 2.581(3) | | |

| | | | | | |
|---|----------|-------------|----------|---------------------------|----------|
| O14 ⁱ —Na1—O15 ⁱⁱ | 103.0(1) | N4—Cu1—O9 | 94.0(1) | O3—Nd1—O7 | 134.6(1) |
| O14 ⁱ —Na1—O15 | 171.2(1) | O5—Cu1—O9 | 94.8(1) | O10—Nd1—O7 | 96.4(1) |
| O15 ⁱⁱ —Na1—O15 | 86.0(1) | O1—Cu1—O9 | 95.3(1) | O11—Nd1—O7 | 69.7(1) |
| O14 ⁱ —Na1—O14 | 87.3(1) | O12—Nd1—O13 | 75.9(1) | N1—Nd1—O7 | 132.8(1) |
| O15 ⁱⁱ —Na1—O14 | 169.7(2) | O12—Nd1—O3 | 69.2(1) | O12—Nd1—O8 ⁱⁱⁱ | 84.9(1) |
| O15—Na1—O14 | 83.8(1) | O13—Nd1—O3 | 70.1(1) | O13—Nd1—O8 ⁱⁱⁱ | 136.1(1) |
| O14 ⁱ —Na1—O16 | 90.6(1) | O12—Nd1—O10 | 138.6(1) | O3—Nd1—O8 ⁱⁱⁱ | 66.2(1) |
| O15 ⁱⁱ —Na1—O16 | 91.7(1) | O13—Nd1—O10 | 141.9(1) | O10—Nd1—O8 ⁱⁱⁱ | 74.6(1) |
| O15—Na1—O16 | 89.0(1) | O3—Nd1—O10 | 129.1(1) | O11—Nd1—O8 ⁱⁱⁱ | 72.1(1) |
| O14—Na1—O16 | 87.0(1) | O12—Nd1—O11 | 71.9(1) | N1—Nd1—O8 ⁱⁱⁱ | 84.0(1) |
| O14 ⁱ —Na1—O17 | 81.9(2) | O13—Nd1—O11 | 134.1(1) | O7—Nd1—O8 ⁱⁱⁱ | 141.3(1) |
| O15 ⁱⁱ —Na1—O17 | 71.4(2) | O3—Nd1—O11 | 124.3(1) | O12—Nd1—N3 | 136.1(1) |
| O15—Na1—O17 | 101.5(2) | O10—Nd1—O11 | 67.8(1) | O13—Nd1—N3 | 75.3(1) |
| O14—Na1—O17 | 111.7(2) | O12—Nd1—N1 | 131.4(1) | O3—Nd1—N3 | 128.2(1) |
| O16—Na1—O17 | 159.2(2) | O13—Nd1—N1 | 80.3(1) | O10—Nd1—N3 | 67.4(1) |
| N2—Cu1—N4 | 97.5(1) | O3—Nd1—N1 | 63.0(1) | O11—Nd1—N3 | 107.5(1) |
| N2—Cu1—O1 | 82.5(1) | O10—Nd1—N1 | 82.3(1) | N1—Nd1—N3 | 74.2(1) |
| N4—Cu1—O5 | 82.7(1) | O11—Nd1—N1 | 145.5(1) | O7—Nd1—N3 | 62.3(1) |
| O1—Cu1—O5 | 96.4(1) | O12—Nd1—O7 | 77.8(1) | O8 ⁱⁱⁱ —Nd1—N3 | 138.0(1) |
| N2—Cu1—O9 | 91.9(1) | O13—Nd1—O7 | 72.3(1) | | |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y, -z+3/2$; (iii) $x, -y+1, z-1/2$.

Table S2. Hydrogen bonding geometry (Å, °)

| Complex 1 | | | | |
|------------------------------|------------|------------|------------|--------------|
| <i>Donor—H…Acceptor</i> | <i>D—H</i> | <i>H…A</i> | <i>D…A</i> | <i>D—H…A</i> |
| O9—H9A…O18 ^{iv} | 0.94 | 2.05 | 2.695(4) | 124 |
| O9—H9B…O2 ⁱⁱⁱ | 0.93 | 2.32 | 2.911(4) | 121 |
| O10—H10A…O6 ^v | 0.93 | 2.12 | 2.875(4) | 138 |
| O10—H10B…O9 | 0.93 | 2.26 | 2.865(4) | 122 |
| O11—H11A…O19 | 0.96 | 2.28 | 3.008(3) | 132 |
| O11—H11B…O6 ^v | 0.96 | 2.53 | 3.475(4) | 168 |
| O12—H12B…O3 ^{vi} | 0.94 | 1.82 | 2.690(4) | 153 |
| O12—H12A…O8 ⁱ | 0.92 | 2.58 | 3.320(4) | 138 |
| O13—H13A…O7 | 0.96 | 2.32 | 2.946(4) | 122 |
| O13—H13B…O1 ^{vii} | 0.96 | 1.80 | 2.744(4) | 168 |
| O14—H14A…O18 ^{viii} | 0.96 | 1.85 | 2.772(5) | 161 |
| O14—H14B…O1 ^{ix} | 0.96 | 1.99 | 2.924(4) | 165 |
| O15—H15A…O5 ^{ix} | 0.96 | 2.48 | 3.303(4) | 144 |
| O15—H15B…O2 ^x | 0.96 | 1.84 | 2.773(4) | 163 |
| O16—H16A…O7 ^{xi} | 0.95 | 2.57 | 3.278(4) | 132 |
| O16—H16B…O8 ^{xi} | 0.95 | 2.30 | 2.908(4) | 121 |
| O17—H17B…O13 ^{vi} | 0.96 | 2.02 | 2.773(6) | 134 |
| O17—H17A…O19 | 0.94 | 2.32 | 2.833(7) | 114 |
| O18—H18A…O8 ^{xii} | 0.96 | 1.68 | 2.632(4) | 173 |
| O18—H18B…O6 | 0.96 | 1.77 | 2.704(4) | 165 |
| O19—H19A…O4 ⁱⁱⁱ | 0.96 | 1.95 | 2.909(4) | 173 |
| O19—H19B…O4 ^{vi} | 0.97 | 1.96 | 2.909(4) | 166 |

Symmetry codes: (i) $-x+1, y, -z+3/2$; (iii) $x, -y+1, z+1/2$; (iv) $x, -y+1, z-1/2$; (v) $-x+1/2, y-1/2, -z+3/2$; (vi) $-x+1, -y+1, -z+1$; (vii) $-x+1/2, -y+3/2, -z+1$; (viii) $x+1/2, -y+1/2, z-1/2$; (ix) $x+1/2, y-1/2, z$; (x) $x+1/2, -y+1/2, z+1/2$; (xi) $-x+1, y-1, -z+3/2$; (xii) $-x+1/2, -y+3/2, -z+2$.

| Complex 2 | | | | |
|------------------------------|------------|------------|------------|--------------|
| <i>Donor—H…Acceptor</i> | <i>D—H</i> | <i>H…A</i> | <i>D…A</i> | <i>D—H…A</i> |
| O9—H9A…O2 ⁱⁱⁱ | 0.96 | 1.94 | 2.884(4) | 169 |
| O9—H9B…O18 | 0.96 | 1.74 | 2.681(4) | 165 |
| O10—H10A…O9 | 0.96 | 1.94 | 2.878(4) | 165 |
| O10—H10B…O6 ^v | 0.96 | 1.88 | 2.838(4) | 176 |
| O11—H11A…O8 ^{iv} | 0.97 | 1.93 | 2.848(4) | 158 |
| O11—H11B…O6 ^v | 0.96 | 2.47 | 3.422(4) | 172 |
| O12—H12B…O8 ^{vi} | 0.97 | 2.50 | 3.269(4) | 136 |
| O12—H12A…O3 ^{vii} | 0.99 | 1.78 | 2.694(4) | 151 |
| O13—H13A…O17 ^{viii} | 0.95 | 1.98 | 2.765(6) | 139 |
| O13—H13B…O1 ^{ix} | 0.95 | 1.99 | 2.745(4) | 135 |
| O14—H14A…O2 ⁱ | 0.96 | 1.88 | 2.775(4) | 155 |
| O14—H14B…O6 ^x | 0.96 | 2.56 | 3.499(4) | 166 |
| O15—H15A…O1 ^{iv} | 0.96 | 2.03 | 2.915(4) | 152 |
| O15—H15B…O18 ^{iv} | 0.97 | 1.79 | 2.745(4) | 165 |
| O16—H16A…O13 ^{xi} | 0.95 | 1.90 | 2.828(4) | 167 |
| O16—H16B…O8 ^{ix} | 0.95 | 1.97 | 2.861(4) | 155 |
| O17—H17A…O5 ^{iv} | 0.95 | 2.09 | 2.826(7) | 133 |
| O17—H17B…O19 ^{xii} | 0.96 | 1.92 | 2.868(6) | 168 |
| O18—H18A…O6 ^{iv} | 0.97 | 1.73 | 2.686(4) | 169 |
| O18—H18B…O8 ^v | 0.96 | 1.69 | 2.634(4) | 169 |
| O19—H19A…O17 ^{viii} | 0.96 | 2.32 | 2.868(6) | 116 |
| O19—H19B…O4 | 0.96 | 1.88 | 2.832(4) | 172 |

Symmetry codes: (i) $-x+1, y, -z+3/2$; (iii) $x, -y+1, z-1/2$; (iv) $x, -y+1, z+1/2$; (v) $-x+1/2, y-1/2, -z+1/2$; (vi) $-x, y, -z+1/2$; (vii) $-x, -y+1, -z+1$; (viii) $-x+1/2, -y+1/2, -z+3/2$; (ix) $-x+1/2, -y+3/2, -z+1$; (x) $-x+1, -y+1, -z+1$; (xi) $x+1/2, -y+3/2, z+1/2$; (xii) $x+1/2, y-1/2, z$.

Complex 3

| <i>Doner</i> —H... <i>Acceptor</i> | D—H | H...A | D...A | D—H...A |
|------------------------------------|------|-------|-----------|---------|
| O9—H9A...O2 ⁱⁱⁱ | 0.95 | 1.94 | 2.891 (5) | 171 |
| O9—H9B...O18 ^v | 0.95 | 1.79 | 2.671 (5) | 151 |
| O10—H10A...O6 ^v | 0.96 | 1.92 | 2.862 (5) | 168 |
| O10—H10B...O9 | 0.96 | 1.92 | 2.876 (5) | 174 |
| O11—H11B...O19 ^{vi} | 0.96 | 2.41 | 2.984 (4) | 118 |
| O11—H11A...O6 ^v | 0.96 | 2.49 | 3.443 (6) | 170 |
| O12—H12A...O3 ^{vii} | 0.96 | 1.76 | 2.703 (5) | 168 |
| O12—H12B...O7 ⁱ | 0.96 | 1.93 | 2.855 (5) | 160 |
| O13—H13B...O1 ^{viii} | 0.94 | 1.92 | 2.748 (5) | 145 |
| O13—H13A...O16 | 0.94 | 2.17 | 2.813 (5) | 125 |
| O14—H14A...O18 ^j | 0.96 | 1.81 | 2.759 (5) | 170 |
| O14—H14B...O1 ^{ix} | 0.96 | 2.02 | 2.920 (5) | 155 |
| O15—H15B...O5 ^x | 0.96 | 2.41 | 3.301 (5) | 155 |
| O15—H15A...O2 ^{viii} | 0.96 | 1.84 | 2.764 (5) | 161 |
| O16—H16B...O8 ⁱ | 0.94 | 2.22 | 2.892 (5) | 128 |
| O16—H16A...O7 ⁱ | 0.94 | 2.57 | 3.291 (5) | 134 |
| O17—H17B...O19 ^{xi} | 0.94 | 1.92 | 2.833 (8) | 162 |
| O17—H17A...O13 ⁱⁱ | 0.95 | 2.18 | 2.766 (8) | 119 |
| O18—H18A...O8 | 0.96 | 1.70 | 2.627 (5) | 162 |
| O18—H18B...O6 ^{xii} | 0.96 | 1.74 | 2.695 (5) | 171 |
| O19—H19A...O4 ⁱ | 0.96 | 1.97 | 2.880 (5) | 158 |
| O19—H19B...O4 ^{xiii} | 0.96 | 1.96 | 2.880 (5) | 161 |

Symmetry codes: (i) $-x+1, y, -z+1/2$; (ii) $-x+1, -y+1, -z$; (iii) $x, -y, z+1/2$; (v) $-x+1/2, y-1/2, -z+1/2$; (vi) $-x+1, -y, -z+1$; (vii) $-x+1, -y, -z$; (viii) $-x+1/2, -y+1/2, -z$; (ix) $x+1/2, y+1/2, z$; (x) $-x+1/2, y+1/2, -z+1/2$; (xi) $-x+1, -y+1, -z+1$; (xii) $-x+1/2, -y+1/2, -z+1$; (xiii) $x, y, z+1$.

Complex 4

| <i>Doner</i> —H... <i>Acceptor</i> | D—H | H...A | D...A | D—H...A |
|------------------------------------|------|-------|-----------|---------|
| O9—H9A...O18 ^v | 0.96 | 1.73 | 2.689 (4) | 173 |
| O9—H9B...O6 ⁱⁱⁱ | 0.96 | 1.98 | 2.907 (4) | 162 |
| O10—H10A...O9 | 0.96 | 1.92 | 2.874 (4) | 171 |
| O10—H10B...O2 ^v | 0.96 | 1.92 | 2.862 (4) | 166 |
| O11—H11A...O19 | 0.96 | 2.42 | 2.971 (3) | 117 |
| O11—H11B...O4 ^{iv} | 0.96 | 1.91 | 2.851 (4) | 166 |
| O12—H12A...O3 ^{vi} | 0.96 | 1.94 | 2.861 (4) | 159 |
| O12—H12B...O7 ^{vii} | 0.96 | 1.76 | 2.700 (4) | 165 |
| O13—H13A...O5 ^{viii} | 0.95 | 2.15 | 2.758 (4) | 121 |
| O13—H13B...O16 ^{ix} | 0.94 | 2.29 | 2.830 (4) | 115 |
| O14—H14A...O5 ⁱⁱⁱ | 0.96 | 2.00 | 2.920 (4) | 161 |
| O14—H14B...O18 ^x | 0.96 | 1.82 | 2.755 (4) | 165 |
| O15—H15A...O6 ⁱⁱⁱ | 0.96 | 1.83 | 2.774 (4) | 165 |
| O15—H15B...O1 | 0.96 | 2.44 | 3.294 (4) | 148 |
| O16—H16B...O4 ^{xi} | 0.95 | 2.16 | 2.885 (4) | 132 |
| O17—H17A...O1 ⁱⁱ | 0.96 | 1.88 | 2.840 (7) | 174 |
| O17—H17B...O19 ^{xii} | 0.96 | 1.91 | 2.849 (7) | 167 |
| O18—H18A...O4 | 0.96 | 1.70 | 2.640 (4) | 167 |
| O18—H18B...O2 ^x | 0.96 | 1.75 | 2.702 (4) | 171 |
| O19—H19B...O12 | 0.96 | 2.57 | 3.491 (6) | 161 |

Symmetry codes: (ii) $-x+1, y, -z+3/2$; (iii) $x, -y+1, z-1/2$; (iv) $x, -y+1, z+1/2$; (v) $-x+1/2, y-1/2, -z+1/2$,

$-z+3/2$; (vi) $-x, y, -z+3/2$; (vii) $-x, -y+1, -z+2$; (viii) $-x+1/2, -y+3/2, -z+2$; (ix) $-x+1/2, y+1/2, -z+3/2$; (x) $-x+1/2, -y+3/2, -z+1$; (xi) $x+1/2, y-1/2, z$; (xii) $x+1/2, y+1/2, z$.
