**Electronic Supplementary Information (ESI)**

# Hydrothermal synthesis, structures, and catalytic performance of five coordination compounds driven by 5-aminoisophthalic acid

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Electronic Supplementary Information (ESI) contains: FTIR spectra (Fig. S1), PXRD patterns (Fig. S2), additional catalysis data (Figs. S3−S6), catalytic mechanism (Scheme S1), structural parameters (Tables S1 and S2). CCDC-2367606–2367610.

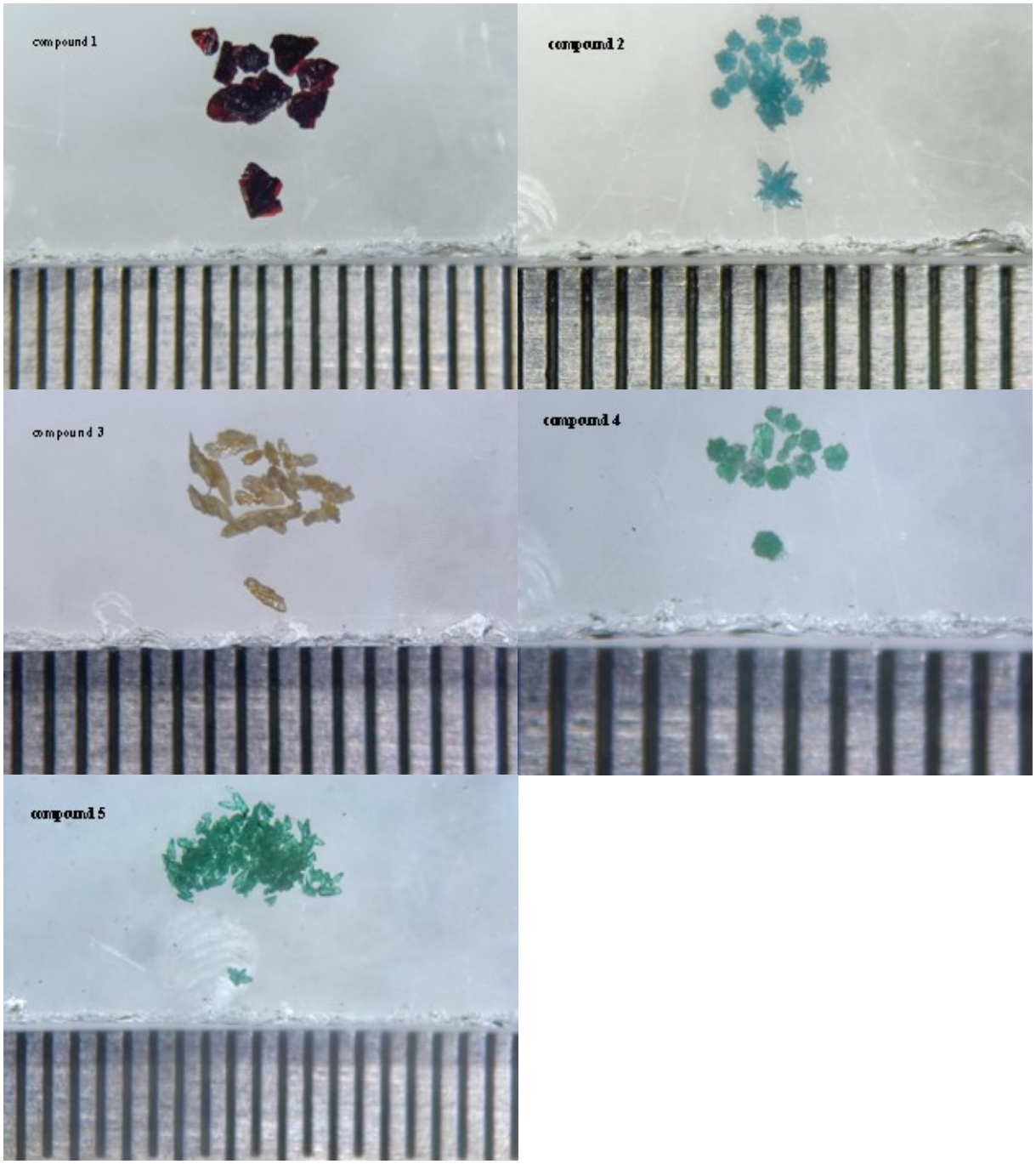
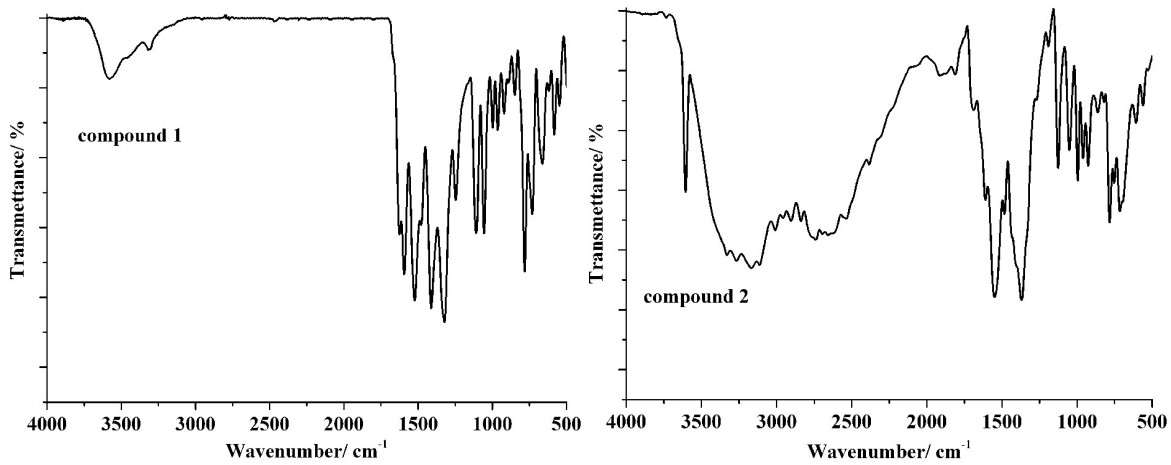



**Fig. S1**. The optical images of compounds **1**–**5**. The minimum scale value is 0.5 mm.



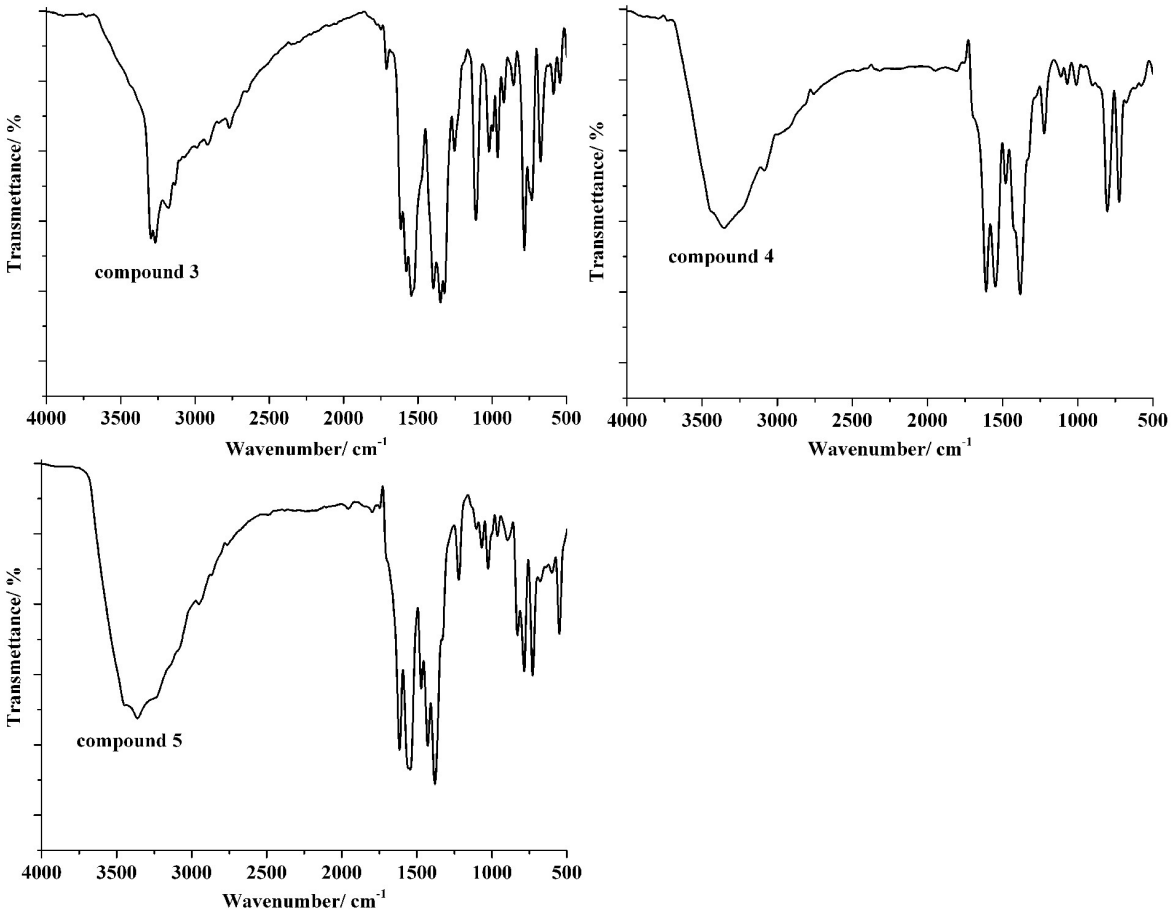
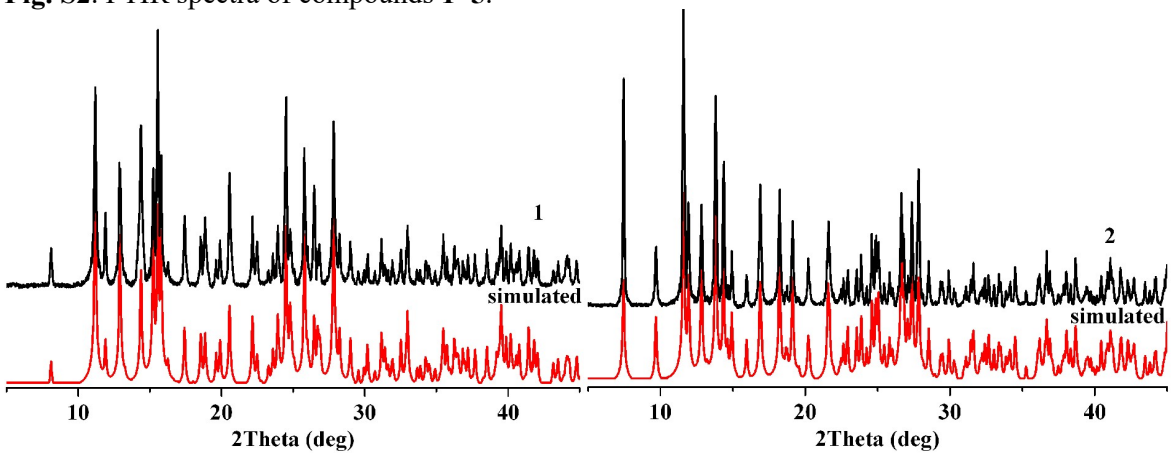



**Fig. S2**. FTIR spectra of compounds **1**–**5**.



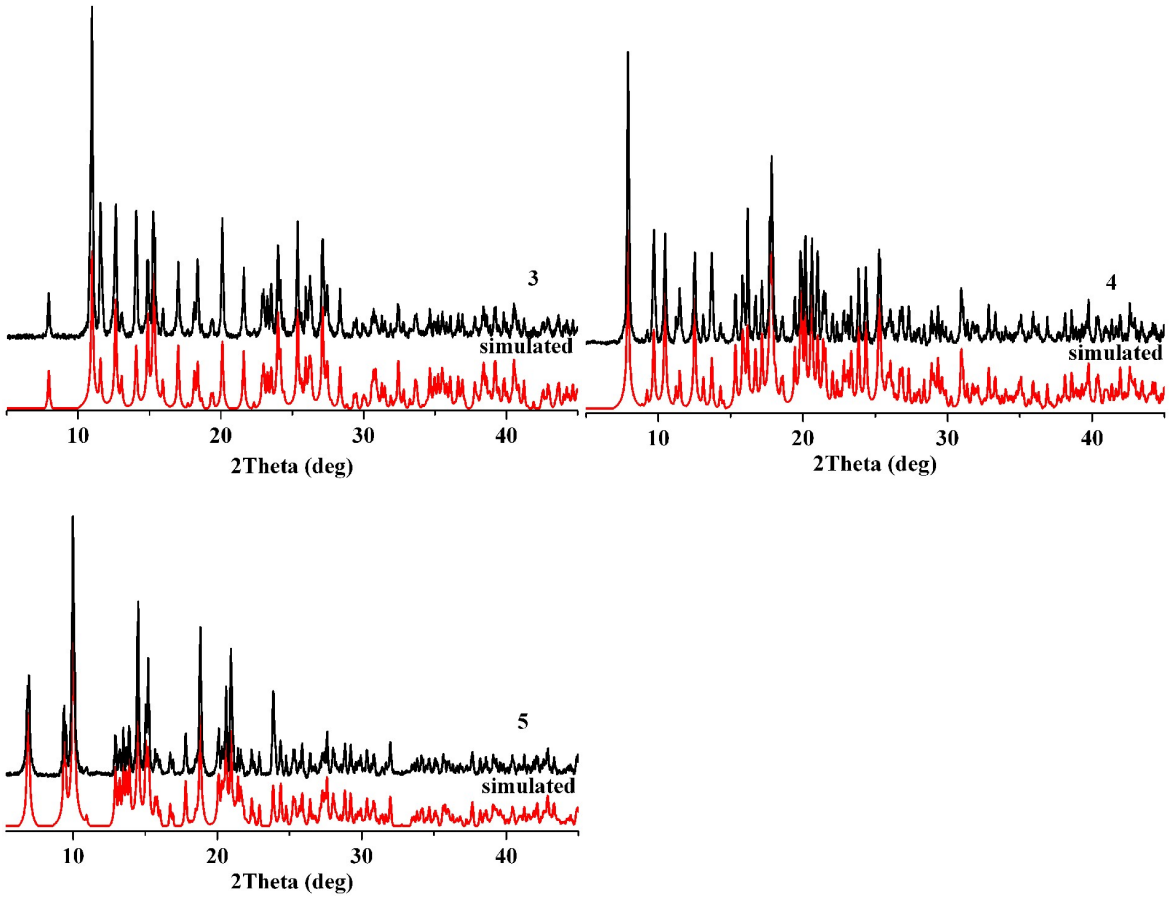



**Fig. S3**. PXRD patterns of compounds **1**–**5** at room temperature. Black paterns correspnond to the experimental data obtained using the as-synthesized bulk samples. Red patterns were simulated from the single crystal X-ray data.

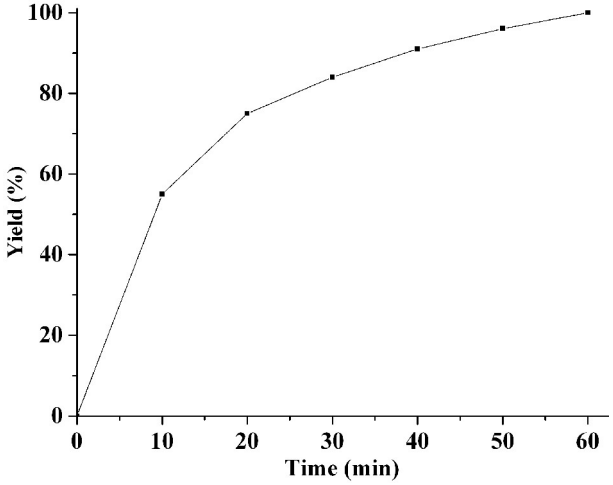



**Fig. S4.** Accumulation of product vs. time in the Knoevenagel reaction of pyridine-3-aldehyde with propanedinitrile catalysed by **3**. Reaction conditions are those of Table 2, entries 1−6.

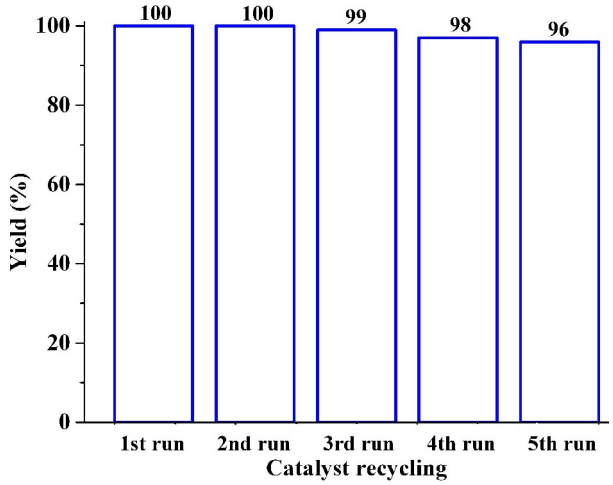



**Fig. S5.** Catalyst recycling experiments in the Knoevenagel reaction of pyridine-3-aldehyde with propanedinitrile catalysed by **3**. Reaction conditions are those of Table 2, entry 6.

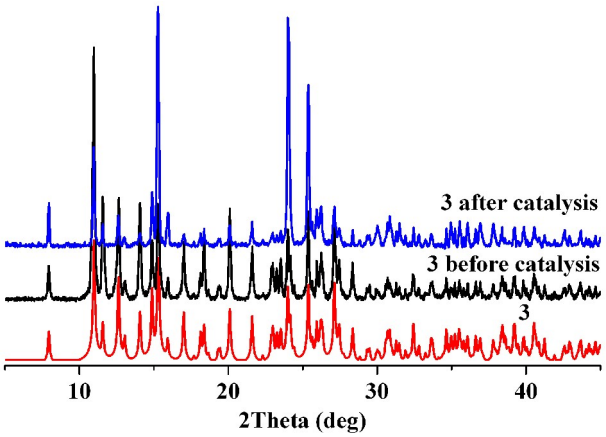



**Fig. S6.** PXRD patterns for **3**: simulated (red), before (black) and after (blue) catalytic experiments.

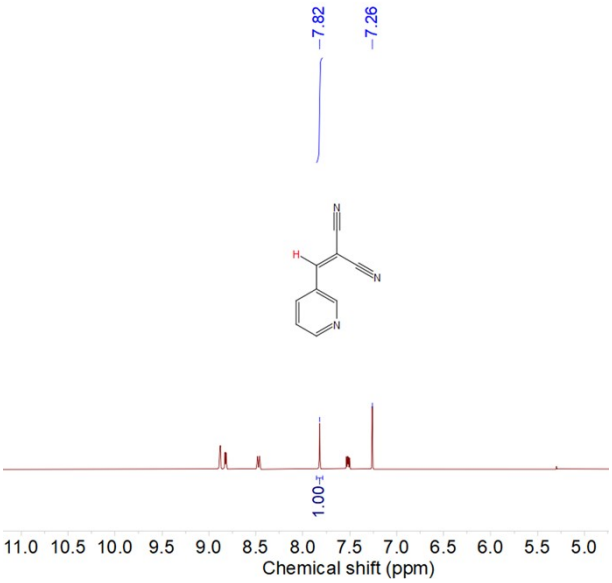
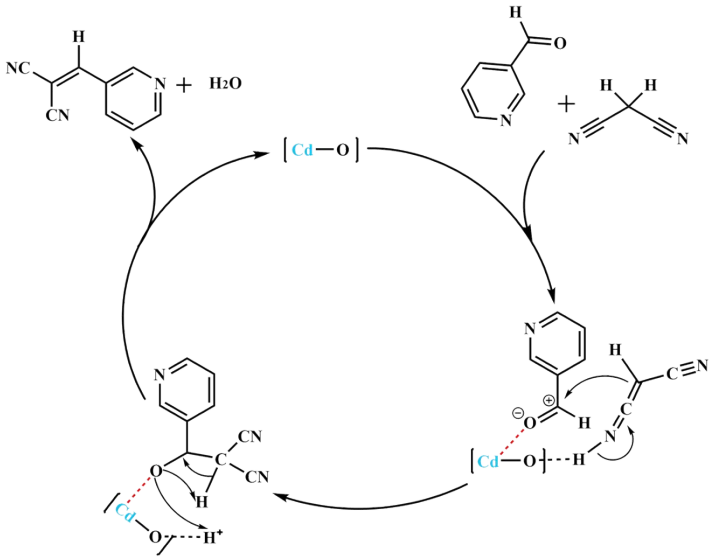



**Fig. S7.** Example of the integration in the $^1$H NMR spectrum of the reaction mixture for the determination of the Knoevenagel reaction product (conditions of Table 2, Entry 6).

**Examples of product yield calculation in the Knoevenagel reaction.** The C(=O) *H* signal of pyridine-3-aldehyde appears at $\delta$10.11 ppm, while product shows a characteristic signal at $\delta$7.82 ppm.
Total integration of both signals: unreacted pyridine-3-aldehyde + product = 0 + 1 = 1.
Percentage of the unreacted substrate: 0/1 = 0
Conversion of pyridine-3-aldehyde = yield of product = 100−0 = 100%.




**Scheme S1.** Plausible mechanism for the Knoevenagel condensation reaction catalyzed by **3**.

**Table S1**. Selected bond lengths [Å] and angles [°] for compounds **1**–**5**.[a]

| **1** | | | | | |
|---|---|---|---|---|---|
| Co(1)–O(1) | 2.044(2) | Co(1)–O(3) | 2.399(2) | Co(1)–O(4)i | 2.111(2) |
| Co(1)–N(1)ii | 2.177(2) | Co(1)–N(2) | 2.087(2) | Co(1)–N(5) | 2.230(3) |
| O(1)–Co(1)–N(2) | 107.07(9) | O(1)–Co(1)–O(4) | 101.69(8) | O(4)i–Co(1)–N(2)i | 145.34(9) |
| O(1)–Co(1)–N(1)ii | 96.55(8) | N(1)ii–Co(1)–N(2) | 104.43(9) | N(1)ii–Co(1)–O(4)i | 90.87(8) |

| | | | | | |
|---|---|---|---|---|---|
| O(1)–Co(1)–N(5) | 91.79(9) | N(2)–Co(1)–N(5) | 76.90(9) | O(4)i–Co(1)–N(5) | 83.36(9) |
| N(1)ii–Co(1)–N(5) | 170.68(9) | O(1)–Co(1)–O(3)i | 159.46(7) | N(2)–Co(1)–O(3)i | 91.89(8) |
| O(4)i–Co(1)–O(3)i | 57.82(7) | O(3)i–Co(1)–N(1)ii | 85.97(8) | O(3)i–Co(1)–N(5) | 84.76(8) |
| | | **2** | | | |
| Ni(1)–O(1) | 2.021(2) | Ni(1)–O(5) | 2.113(2) | Ni(1)–O(6) | 2.120(2) |
| Ni(1)–N(1)i | 2.164(2) | Ni(1)–N(2) | 2.072(2) | Ni(1)–N(5) | 2.102(2) |
| O(1)–Ni(1)–N(2) | 93.09(7) | O(1)–Ni(1)–N(5) | 172.95(7) | N(5)–Ni(1)–N(2) | 80.37(7) |
| O(1)–Ni(1)–O(5) | 90.45(7) | O(5)–Ni(1)–N(2) | 176.25(7) | O(5)–Ni(1)–N(5) | 96.14(7) |
| O(1)–Ni(1)–O(6) | 90.13(7) | O(6)–Ni(1)–N(2) | 90.17(7) | O(6)–Ni(1)–N(5) | 87.28(7) |
| O(5)–Ni(1)–O(6) | 91.05(7) | O(1)–Ni(1)–N(1)i | 87.87(7) | N(1)i–Ni(1)–N(2) | 91.90(7) |
| N(1)i–Ni(1)–N(5) | 94.94(7) | N(1)i–Ni(1)–O(5) | 87.00(7) | N(1)i–Ni(1)–O(6) | 177.19(7) |
| | | **3** | | | |
| Cd(1)–O(2) | 2.248(2) | Cd(1)–O(3)i | 2.285(2) | Cd(1)–N(1)ii | 2.341(2) |
| Cd(1)–N(2) | 2.257(2) | Cd(1)–N(5) | 2.447(3) | | |
| O(2)–Cd(1)–N(2) | 114.04(9) | O(2)–Cd(1)–O(3)i | 99.45(7) | O(3)i–Cd(1)–N(2) | 137.41(8) |
| O(2)–Cd(1)–N(1)ii | 99.62(8) | N(1)ii–Cd(1)–N(2) | 108.28(9) | O(3)i–Cd(1)–N(1)ii | 90.25(8) |
| O(2)–Cd(1)–N(5) | 92.92(8) | N(2)–Cd(1)–N(5) | 72.01(9) | O(3)i–Cd(1)–N(5) | 81.12(9) |
| N(1)ii–Cd(1)–N(5) | 165.82(9) | | | | |
| | | **4** | | | |
| Ni(1)–O(1) | 2.052(2) | Ni(1)–O(2) | 2.192(2) | Ni(1)–O(3)i | 2.133(2) |
| Ni(1)–O(4)i | 2.082(2) | Ni(1)–N(2) | 2.050(2) | Ni(1)–N(3)ii | 2.062(2) |
| N(2)–Ni(1)–O(1) | 95.11(6) | N(2)–Ni(1)–N(3)ii | 97.29(6) | N(3)ii–Ni(1)–O(1) | 98.32(6) |
| N(2)–Ni(1)–O(4)i | 158.56(6) | O(4)i–Ni(1)–O(1) | 104.09(5) | N(3)ii–Ni(1)–O(4)i | 89.39(6) |
| N(2)–Ni(1)–O(3)i | 96.61(6) | O(1)–Ni(1)–O(3)i | 161.86(5) | N(3)ii–Ni(1)–O(3)i | 93.88(6) |
| O(4)i–Ni(1)–O(3)i | 62.50(5) | N(2)–Ni(1)–O(2) | 90.03(6) | O(2)–Ni(1)–O(1) | 62.03(5) |
| N(3)ii–Ni(1)–O(2) | 159.68(6) | O(4)i–Ni(1)–O(2) | 90.62(5) | O(3)i–Ni(1)–O(2) | 104.13(5) |
| | | **5** | | | |
| Ni(1)–O(2) | 2.002(3) | Ni(1)–O(3)i | 2.106(3) | Ni(1)–O(4)i | 2.160(3) |
| Ni(1)–O(13) | 2.059(4) | Ni(1)–N(4) | 2.089(4) | Ni(1)–N(5)ii | 2.081(4) |
| Ni(2)–O(6) | 2.014(3) | Ni(2)–O(7)iii | 2.093(3) | Ni(2)–O(8)iii | 2.158(4) |
| Ni(2)–N(1) | 2.145(4) | Ni(2)–N(6) | 2.078(4) | Ni(2)–N(7)iv | 2.124(4) |
| Ni(3)–O(9) | 2.019(3) | Ni(3)–O(11)i | 2.115(4) | Ni(3)–O(12)i | 2.107(3) |
| Ni(3)–O(14) | 2.070(4) | Ni(3)–N(8) | 2.078(4) | Ni(3)–N(9)v | 2.109(5) |
| 2.109(5) | 93.44(15) | O(2)–Ni(1)–N(5)ii | 90.43(15) | O(13)–Ni(1)–N(5)ii | 92.65(16) |
| O(2)–Ni(1)–N(4) | 88.82(15) | O(13)–Ni(1)–N(4) | 89.58(16) | N(4)–Ni(1)–N(5)ii | 177.69(19) |
| O(3)i–Ni(1)–O(2) | 162.19(14) | O(13)–Ni(1)–O(3)i | 104.24(15) | O(3)i–Ni(1)–N(5)ii | 90.93(15) |
| O(3)i–Ni(1)–N(4) | 89.12(16) | O(4)i–Ni(1)–O(2) | 100.50(13) | O(4)i–Ni(1)–O(13) | 165.66(13) |
| O(4)i–Ni(1)–N(5)ii | 90.62(15) | O(4)i–Ni(1)–N(4) | 87.37(15) | O(3)i–Ni(1)–O(4)i | 61.73(13) |
| O(6)–Ni(2)–N(6) | 89.28(16) | O(6)–Ni(2)–O(7)iii | 163.45(16) | O(7)iii–Ni(2)–N(6) | 88.47(16) |
| O(6)–Ni(2)–N(7)iv | 88.52(16) | N(6)–Ni(2)–O(7)iii | 175.46(18) | N(7)iv–Ni(2)–O(7)iii | 92.51(15) |
| O(6)–Ni(2)–N(1) | 100.05(17) | N(6)–Ni(2)–N(1) | 90.81(18) | N(1)–Ni(2)–O(7)iii | 96.38(15) |
| N(7)iv–Ni(2)–N(1) | 93.49(17) | O(6)–Ni(2)–O(8)iii | 101.45(15) | N(6)–Ni(2)–O(8)iii | 87.41(17) |

| | | | | | |
|---|---|---|---|---|---|
| O(7)iii–Ni(2)–O(8)iii | 62.07(13) | N(7)iv–Ni(2)–O(8)iii | 89.12(16) | N(1)–Ni(2)–O(8)iii | 158.40(15) |
| O(9)–Ni(3)–O(14) | 95.76(16) | O(9)–Ni(3)–N(8) | 90.04(16) | N(8)–Ni(3)–O(14) | 90.14(17) |
| O(9)–Ni(3)–O(12)i | 162.82(16) | O(12)i–Ni(3)–O(14) | 101.39(17) | N(8)–Ni(3)–O(12)i | 88.86(17) |
| O(9)–Ni(3)–N(9)v | 89.96(17) | O(14)–Ni(3)–N(9)v | 90.46(17) | N(9)v–Ni(3)–N(8) | 179.4(2) |
| O(12)i–Ni(3)–N(9)v | 90.97(17) | O(9)–Ni(3)–O(11)i | O(9)–Ni(3) | O(14)–Ni(3)–O(11)i | 163.61(15) |
| N(8)–Ni(3)–O(11)i | 89.61(17) | O(11)i–Ni(3)–O(12)i | 62.21(15) | N(9)v–Ni(3)–O(11)i | 89.81(17) |

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

**Table S2**. Hydrogen bonds in crystal packing [Å, °] of **1**–**5**.

| Compound | D–H···A | *d*(D–H) | *d*(H···A) | *d*(D···A) | ∠DHA | Symmetry code |
|---|---|---|---|---|---|---|
| **1** | N(1)–H(1A)···O(2) | 0.890 | 2.466 | 3.213 | 141.88 | –*x*, –*y*, –*z* + 2 |
| | N(1)–H(1B)···O(4) | 0.890 | 2.123 | 2.943 | 152.99 | –*x* – 1, –*y* + 1, –*z* + 2 |
| | N(3)–H(1)···O(3) | 0.860 | 1.979 | 2.735 | 146.05 | –*x* + 1, –*y* + 1, –*z* + 1 |
| | N(4)–H(2)···O(1) | 0.860 | 2.274 | 2.989 | 140.56 | –*x* + 1, –*y* , –*z* + 1 |
| **2** | N(1)–H(5A)···O(7) | 0.890 | 2.282 | 3.144 | 162.85 | |
| | N(1)–H(5B)···O(8) | 0.890 | 2.258 | 3.117 | 162.09 | –*x* + 1, –*y* + 1, –*z* + 1 |
| | N(3)–H(1)···O(4) | 0.860 | 1.861 | 2.717 | 172.86 | *x* – 1, *y* + 1, *z* |
| | N(4)–H(2)···O(3) | 0.860 | 1.814 | 2.674 | 179.13 | *x* – 1, *y* + 1, *z* |
| | O(5)–H(1W)···O(2) | 0.852 | 1.915 | 2.667 | 146.39 | |
| | O(5)–H(2W)···O(2) | 0.853 | 1.954 | 2.785 | 164.74 | –*x* + 1, *y* + 1/2, –*z* + 3/2 |
| | O(6)–H(3W)···O(8) | 0.852 | 2.135 | 2.913 | 151.49 | |
| | O(6)–H(4W)···O(4) | 0.852 | 1.902 | 2.738 | 166.76 | –*x* + 1, *y* + 1, –*z* + 1 |
| | O(7)–H(5W)···O(5) | 0.850 | 1.938 | 2.774 | 167.82 | *x* , –*y* + 3/2, *z* – 1/2 |
| | O(7)–H(6W)···O(3) | 0.850 | 1.879 | 2.729 | 179.57 | –*x* + 1, –*y* + 1, –*z* + 1 |
| | O(8)–H(7W)···N(5) | 0.850 | 2.644 | 3.232 | 129.43 | *x*, *y* – 1, *z* |
| | O(8)–H(8W)···O(7) | 0.850 | 1.844 | 2.664 | 161.47 | *x* , –*y* + 3/2, *z* + 1/2 |
| **3** | N(1)–H(1A)···O(2) | 0.890 | 2.324 | 3.118 | 148.56 | –*x* + 2, –*y* +2, –*z* |
| | N(1)–H(1B)···O(3) | 0.890 | 2.133 | 2.934 | 149.27 | –*x* + 3, –*y* +1, –*z* |
| | N(3)–H(1)···O(4) | 0.860 | 1.982 | 2.743 | 146.97 | –*x* + 1, –*y* + 1, –*z* + 1 |
| | N(4)–H(2)···O(2) | 0.860 | 2.278 | 2.991 | 140.39 | –*x* + 1, –*y* + 2, –*z* + 1 |
| **4** | N(1)–H(1A)···O(5) | 0.862 | 2.211 | 2.975 | 147.75 | *x* + 1, *y*, *z* |
| | O(5)–H(1W)···N(4) | 0.850 | 2.050 | 2.891 | 170.00 | *x*, *y*, *z* + 1 |
| | O(5)–H(2W)···O(1) | 0.850 | 1.925 | 2.767 | 170.30 | *x* – 1/2, –*y* + 3/2, *z* + 1/2 |
| **5** | N(1)–H(1B)···O(5) | 0.890 | 2.180 | 2.919 | 140.15 | |
| | O(13)–H(2W)···O(1) | 0.872 | 1.919 | 2.661 | 142.05 | |
| | O(14)–H(4W)···O(10) | 0.884 | 1.877 | 2.634 | 142.63 | |