Supporting information

Quasi – isostructural Co(II) and Ni(II) complexes with mefenamic acid: synthesis, characterization and biological activity

Michał Gacki [1]*, Karolina Kafarska [1], Anna Pietrzak [1], Izabela Korona–Głowniak [2], Wojciech M. Wolf [1]

[1] Institute of General and Ecological Chemistry, Faculty of Chemistry, Lodz University of Technology, 116 Zeromskiego Street, 90-924 Lodz, Poland;
[2] Department of Pharmaceutical Microbiology, Medical University of Lublin, Chodzki 1, 20-093 Lublin, Poland

* Correspondence: michal.gacki@edu.p.lodz.pl;

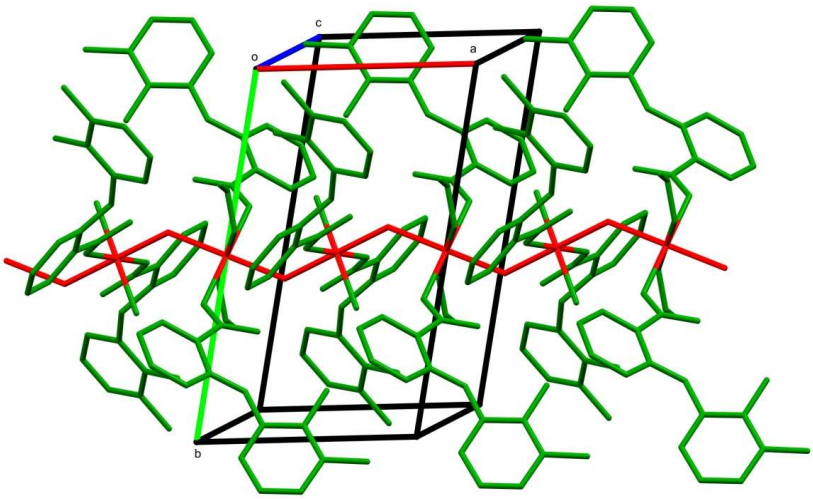

Figure S1. Polymeric chain (in red) running along the [100] axis in **2**. Hydrogen atoms are omitted for clarity.

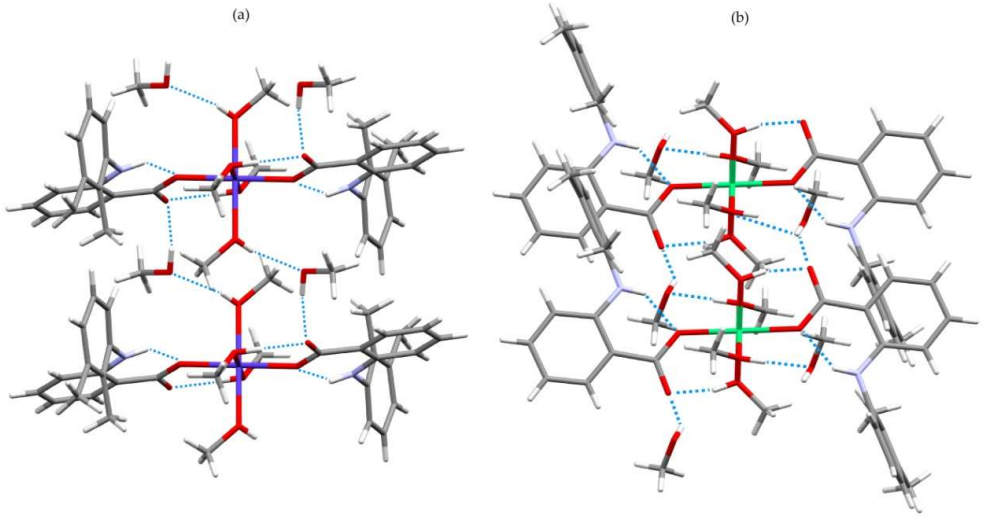

Figure S2. Fragment of the intermolecular chain along [100] stabilized by hydrogen bonds as in **3**(a) and **4**(b). Hydrogens atom are omitted for clarity.

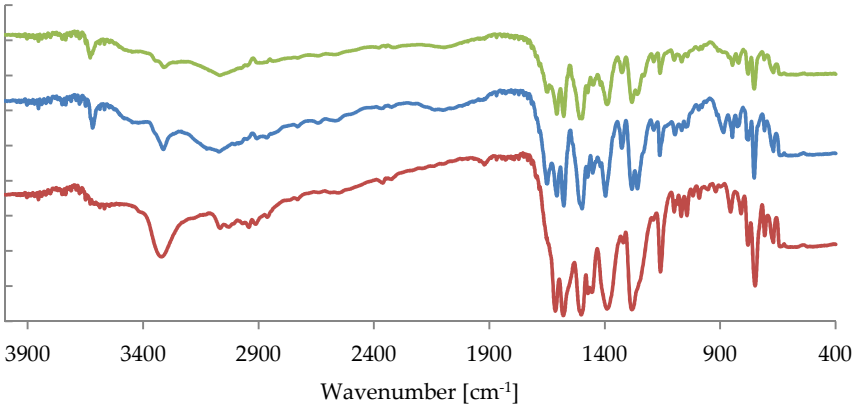

Figure S3. FTIR spectra of **2** (red line), **3** (green line) and **4** (blue line).

Table S1. Bond distances for **2** (Å)

Co1-O1	2.0667(16)	O7 -H6	0.83(3)
Co1-O5	2.1518(15)	C1 -C2	1.381(3)
Co1-O7	2.0748(16)	C1 -C6	1.403(3)
Co1-O1_b	2.0667(16)	N1 -H1	0.90(3)
Co1-O5_b	2.1518(15)	C2 -C3	1.388(4)
Co1-O7_b	2.0748(16)	N2A-H2A	0.84(6)
Co2-O3	2.0454(15)	N2B-H2B	0.83(8)
Co2-O5	2.1493(15)	C3 -C4	1.385(3)
Co2-O6	2.0973(17)	C4 -C5	1.402(3)
Co2-O3_a	2.0454(15)	C5 -C6	1.423(3)
Co2-O5_a	2.1493(15)	C6 -C7	1.486(3)
Co2-O6_a	2.0973(17)	C8 -C9	1.399(3)
O1 -C7	1.277(3)	C8 -C13	1.408(3)
O2 -C7	1.264(3)	C9 -C10	1.388(4)
O3 -C16	1.284(3)	C10-C11	1.379(3)
O4 -C16	1.261(3)	C11-C12	1.399(3)
O7 -C31A	1.435(9)	C12-C14	1.510(3)
O7 -C31B	1.46(2)	C12-C13	1.402(3)
N1 -C5	1.385(3)	C13-C15	1.505(3)
N1 -C8	1.401(3)	C16-C17	1.486(3)
N2A-C22	1.40(2)	C17-C18B	1.437(11)
N2A-C23A	1.51(2)	C17-C18A	1.390(7)
N2B-C22	1.38(3)	C17-C22	1.390(3)
N2B-C23B	1.31(3)	C18A -C19A	1.389(9)
O5 -H5B	0.85(2)	C18B -C19B	1.375(14)
O5 -H5A	0.835(18)	C19A -C20A	1.390(10)
O6 -H6B	0.85(3)	C19B -C20B	1.390(15)
O6 -H6A	0.83(2)	C20A -C21A	1.390(14)
C20B -C21B	1.37(2)	C14-H14A	0.9600
C21A -C22	1.390(5)	C14-H14B	0.9600

C21B -C22	1.455(10)	C14-H14C	0.9600
C23A -C24A	1.390(14)	C15-H15B	0.9600
C23A -C28A	1.391(17)	C15-H15C	0.9600
C23B -C24B	1.39(3)	C15-H15A	0.9600
C23B -C28B	1.39(2)	C18A -H18A	0.9300
C24A -C25A	1.391(12)	C18B -H18B	0.9300
C24B -C25B	1.39(2)	C19A -H19A	0.9300
C25A -C26A	1.390(15)	C19B -H19B	0.9300
C25B -C26B	1.39(2)	C20A -H20A	0.9300
C26A -C27A	1.391(16)	C20B -H20B	0.9300
C26B -C27B	1.39(2)	C21A -H21A	0.9300
C27A -C29A	1.51(3)	C21B -H21B	0.9300
C27A -C28A	1.390(18)	C24A -H24A	0.9300
C27B -C29B	1.51(4)	C24B -H24B	0.9300
C27B -C28B	1.389(19)	C25A -H25A	0.9300
C28A -C30A	1.52(2)	C25B -H25B	0.9300
C28B -C30B	1.53(3)	C26A -H26A	0.9300
C31A -C32A	1.492(16)	C26B -H26B	0.9300
C31B -C32B	1.49(3)	C29A -H29A	0.9600
C1 -H1A	0.9300	C29A -H29B	0.9600
C2 -H2	0.9300	C29A -H29C	0.9600
C3 -H3	0.9300	C29B -H29D	0.9600
C4 -H4	0.9300	C29B -H29E	0.9700
C9 -H9	0.9300	C29B -H29F	0.9600
C10-H10	0.9300	C30A -H30C	0.9600
C11-H11	0.9300	C30A -H30A	0.9600
C30A -H30B	0.9600	C31B -H31D	0.9700
C30B -H30D	0.9600	C32A -H32B	0.9600
C30B -H30E	0.9600	C32A -H32C	0.9600
C30B -H30F	0.9600	C32A -H32A	0.9600
C31A -H31A	0.9700	C32B -H32D	0.9600
C31A -H31B	0.9700	C32B -H32E	0.9600
C31B -H31C	0.9700	C32B -H32F	0.9600

Table S2. Bond angles for **2**, (°)

O1-Co1-O5	90.63(6)	O3_a-Co2-O6_a	88.17(7)
O1-Co1-O7	87.88(7)	O5_a-Co2-O6_a	91.19(6)
O1-Co1-O1_b	180.00	Co1-O1-C7	125.25(14)
O1-Co1-O5_b	89.37(6)	Co2-O3-C16	127.75(14)
O1-Co1-O7_b	92.12(7)	Co1-O5-Co2	130.31(8)
O5-Co1-O7	86.12(6)	Co1-O7-C31A	121.8(4)
O1_b-Co1-O5	89.37(6)	Co1-O7-C31B	134.3(9)
O5-Co1-O5_b	180.00	C5-N1-C8	130.5(2)
O5-Co1-O7_b	93.89(6)	C22-N2A-C23A	122.5(16)
O1_b-Co1-O7	92.12(7)	C22-N2B-C23B	126(2)
O5_b-Co1-O7	93.89(6)	Co1-O5-H5A	109.0(17)
O7-Co1-O7_b	180.00	Co1-O5-H5B	98.1(16)

O1_b-Co1-O5_b	90.63(6)	H5A-O5-H5B	112(2)
O1_b-Co1-O7_b	87.88(7)	Co2-O5-H5B	109.8(16)
O5_b-Co1-O7_b	86.12(6)	Co2-O5-H5A	97.9(17)
O3-Co2-O5	87.42(6)	Co2-O6-H6B	118.9(17)
O3-Co2-O6	88.17(7)	Co2-O6-H6A	115.2(19)
O3-Co2-O3_a	180.00	H6A-O6-H6B	107(3)
O3-Co2-O5_a	92.58(6)	Co1-O7-H6	113.4(19)
O3-Co2-O6_a	91.83(7)	C31A-O7-H6	108(2)
O5-Co2-O6	91.19(6)	C31B-O7-H6	106(2)
O3_a-Co2-O5	92.58(6)	C8-N1-H1	119.1(19)
O5-Co2-O5_a	180.00	C2-C1-C6	121.7(2)
O5-Co2-O6_a	88.82(6)	C5-N1-H1	110.0(19)
O3_a-Co2-O6	91.83(7)	C1-C2-C3	118.7(2)
O5_a-Co2-O6	88.82(6)	C22-N2A-H2A	121(5)
O6-Co2-O6_a	180.00	C23A-N2A-H2A	116(5)
O3_a-Co2-O5_a	87.42(6)	C22-N2B-H2B	111(7)
C23B-N2B-H2B	123(7)	C18A-C17-C22	120.0(2)
C2-C3-C4	121.3(2)	C16-C17-C22	122.1(2)
C3-C4-C5	120.9(2)	C16-C17-C18A	117.9(2)
N1-C5-C6	118.7(2)	C18B-C17-C22	120.2(3)
N1-C5-C4	123.1(2)	C17-C18A-C19A	120.0(6)
C4-C5-C6	118.1(2)	C17-C18B-C19B	122.3(8)
C1-C6-C5	119.3(2)	C18A-C19A-C20A	120.0(10)
C1-C6-C7	117.7(2)	C18B-C19B-C20B	117.3(12)
C5-C6-C7	122.9(2)	C19A-C20A-C21A	120.0(7)
O1-C7-O2	122.6(2)	C19B-C20B-C21B	122.6(10)
O2-C7-C6	119.7(2)	C20A-C21A-C22	120.0(3)
O1-C7-C6	117.7(2)	C20B-C21B-C22	121.2(7)
N1-C8-C9	122.7(2)	N2B-C22-C17	125.2(11)
C9-C8-C13	120.4(2)	C17-C22-C21B	116.4(5)
N1-C8-C13	116.8(2)	C17-C22-C21A	120.0(3)
C8-C9-C10	119.6(2)	N2B-C22-C21B	117.3(12)
C9-C10-C11	120.5(2)	N2A-C22-C17	119.3(9)
C10-C11-C12	120.7(2)	N2A-C22-C21A	119.9(9)
C11-C12-C13	119.6(2)	N2A-C23A-C28A	124.9(13)
C11-C12-C14	119.7(2)	N2A-C23A-C24A	115.1(12)
C13-C12-C14	120.7(2)	C24A-C23A-C28A	120.0(9)
C8-C13-C12	119.2(2)	N2B-C23B-C24B	122.1(18)
C8-C13-C15	119.7(2)	C24B-C23B-C28B	119.9(11)
C12-C13-C15	121.2(2)	N2B-C23B-C28B	117.8(18)
O3-C16-C17	117.9(2)	C23A-C24A-C25A	120.0(9)
O3-C16-O4	122.6(2)	C23B-C24B-C25B	119.9(15)
O4-C16-C17	119.59(19)	C24A-C25A-C26A	120.0(10)
C16-C17-C18B	117.5(3)	C24B-C25B-C26B	120.3(18)
C25A-C26A-C27A	120.0(10)	C12-C11-H11	120.00
C25B-C26B-C27B	119.8(12)	C10-C11-H11	120.00
C28A-C27A-C29A	118.2(15)	C12-C14-H14C	109.00
C26A-C27A-C28A	120.0(10)	C12-C14-H14A	109.00

C26A-C27A-C29A	121.7(15)	C12-C14-H14B	110.00
C28B-C27B-C29B	125(2)	H14B-C14-H14C	109.00
C26B-C27B-C29B	115.1(19)	H14A-C14-H14C	109.00
C26B-C27B-C28B	120.1(12)	H14A-C14-H14B	109.00
C23A-C28A-C30A	117.8(12)	C13-C15-H15B	109.00
C23A-C28A-C27A	120.0(10)	C13-C15-H15A	109.00
C27A-C28A-C30A	122.1(12)	H15A-C15-H15C	109.00
C23B-C28B-C27B	120.1(12)	C13-C15-H15C	109.00
C23B-C28B-C30B	122.0(15)	H15A-C15-H15B	109.00
C27B-C28B-C30B	117.9(15)	H15B-C15-H15C	109.00
O7-C31A-C32A	110.7(7)	C19A-C18A-H18A	120.00
O7-C31B-C32B	116.1(16)	C17-C18A-H18A	120.00
C6-C1-H1A	119.00	C19B-C18B-H18B	119.00
C2-C1-H1A	119.00	C17-C18B-H18B	119.00
C1-C2-H2	121.00	C20A-C19A-H19A	120.00
C3-C2-H2	121.00	C18A-C19A-H19A	120.00
C4-C3-H3	119.00	C20B-C19B-H19B	121.00
C2-C3-H3	119.00	C18B-C19B-H19B	121.00
C3-C4-H4	120.00	C21A-C20A-H20A	120.00
C5-C4-H4	120.00	C19A-C20A-H20A	120.00
C10-C9-H9	120.00	C19B-C20B-H20B	119.00
C8-C9-H9	120.00	C21B-C20B-H20B	119.00
C11-C10-H10	120.00	C20A-C21A-H21A	120.00
C9-C10-H10	120.00	C22-C21A-H21A	120.00
C22-C21B-H21B	119.00	H30A-C30A-H30B	110.00
C20B-C21B-H21B	119.00	C28A-C30A-H30B	109.00
C23A-C24A-H24A	120.00	H30B-C30A-H30C	110.00
C25A-C24A-H24A	120.00	H30A-C30A-H30C	110.00
C23B-C24B-H24B	120.00	C28B-C30B-H30E	109.00
C25B-C24B-H24B	120.00	C28B-C30B-H30D	109.00
C24A-C25A-H25A	120.00	H30D-C30B-H30E	109.00
C26A-C25A-H25A	120.00	H30D-C30B-H30F	110.00
C24B-C25B-H25B	120.00	C28B-C30B-H30F	109.00
C26B-C25B-H25B	120.00	H30E-C30B-H30F	110.00
C25A-C26A-H26A	120.00	O7-C31A-H31A	110.00
C27A-C26A-H26A	120.00	O7-C31A-H31B	110.00
C25B-C26B-H26B	120.00	C32A-C31A-H31A	109.00
C27B-C26B-H26B	120.00	C32A-C31A-H31B	109.00
C27A-C29A-H29A	109.00	H31A-C31A-H31B	108.00
C27A-C29A-H29B	109.00	O7-C31B-H31C	108.00
C27A-C29A-H29C	110.00	O7-C31B-H31D	108.00
H29A-C29A-H29B	109.00	C32B-C31B-H31C	108.00
H29A-C29A-H29C	110.00	H31C-C31B-H31D	107.00
H29B-C29A-H29C	109.00	C32B-C31B-H31D	109.00
C27B-C29B-H29F	110.00	C31A-C32A-H32B	109.00
C27B-C29B-H29D	110.00	C31A-C32A-H32C	109.00
C27B-C29B-H29E	109.00	H32A-C32A-H32C	109.00
H29E-C29B-H29F	109.00	H32B-C32A-H32C	110.00

H29D-C29B-H29E	109.00	H32A-C32A-H32B	110.00
H29D-C29B-H29F	110.00	C31A-C32A-H32A	109.00
C28A-C30A-H30A	109.00	C31B-C32B-H32D	110.00
C28A-C30A-H30C	109.00	C31B-C32B-H32E	109.00
C31B-C32B-H32F	109.00	H32D-C32B-H32F	110.00
H32D-C32B-H32E	109.00	H32E-C32B-H32F	109.00

Table S3. Torsion angles for **2**, (°)

O5-Co1-O1-C7	-29.36(17)	C5-C6-C7-O2	20.9(3)
O7-Co1-O1-C7	56.73(17)	N1-C8-C9-C10	-177.8(2)
O5_b-Co1-O1-C7	150.65(17)	C13-C8-C9-C10	-1.8(4)
O7_b-Co1-O1-C7	-123.27(17)	N1-C8-C13-C12	176.6(2)
O1-Co1-O5-Co2	126.96(10)	N1-C8-C13-C15	-2.5(3)
O7-Co1-O5-Co2	39.12(10)	C9-C8-C13-C12	0.4(3)
O1_b-Co1-O5-Co2	-53.05(10)	C9-C8-C13-C15	-178.8(2)
O7_b-Co1-O5-Co2	-140.88(10)	C8-C9-C10-C11	1.6(4)
O1-Co1-O7-C31A	140.0(4)	C9-C10-C11-C12	0.0(4)
O5-Co1-O7-C31A	-129.2(4)	C10-C11-C12-C13	-1.4(4)
O1_b-Co1-O7-C31A	-40.0(4)	C10-C11-C12-C14	179.5(2)
O5_b-Co1-O7-C31A	50.8(4)	C11-C12-C13-C8	1.2(4)
O5-Co2-O3-C16	-176.26(19)	C11-C12-C13-C15	-179.7(2)
O6-Co2-O3-C16	-84.99(19)	C14-C12-C13-C8	-179.7(2)
O5_a-Co2-O3-C16	3.74(19)	C14-C12-C13-C15	-0.5(4)
O6_a-Co2-O3-C16	95.01(19)	O3-C16-C17-C18A	-20.1(4)
O3-Co2-O5-Co1	-59.60(10)	O3-C16-C17-C22	163.1(2)
O6-Co2-O5-Co1	-147.71(10)	O4-C16-C17-C18A	159.4(4)
O3_a-Co2-O5-Co1	120.40(10)	O4-C16-C17-C22	-17.5(3)
O6_a-Co2-O5-Co1	32.29(10)	C16-C17-C18A-C19A	-176.9(7)
Co1-O1-C7-O2	35.5(3)	C22-C17-C18A-C19A	-0.1(9)
Co1-O1-C7-C6	-143.00(16)	C16-C17-C22-N2A	7.1(12)
Co2-O3-C16-O4	-16.0(3)	C16-C17-C22-C21A	176.8(4)
Co2-O3-C16-C17	163.38(15)	C18A-C17-C22-N2A	-169.7(12)
Co1-O7-C31A-C32A	-157.1(5)	C18A-C17-C22-C21A	0.0(6)
C8-N1-C5-C4	-6.9(4)	C17-C18A-C19A-C20A	0.1(14)
C8-N1-C5-C6	174.2(2)	C18A-C19A-C20A-C21A	0.0(17)
C5-N1-C8-C9	-35.5(4)	C19A-C20A-C21A-C22	0.0(15)
C5-N1-C8-C13	148.4(3)	C20A-C21A-C22-N2A	169.6(13)
C23A-N2A-C22-C17	-166.7(13)	C20A-C21A-C22-C17	0.0(9)
C23A-N2A-C22-C21A	24(2)	N2A-C23A-C24A-C25A	179.0(13)
C22-N2A-C23A-C24A	-114.5(18)	C28A-C23A-C24A-C25A	0.0(15)
C22-N2A-C23A-C28A	64(2)	N2A-C23A-C28A-C27A	-178.8(15)
C6-C1-C2-C3	-0.2(4)	N2A-C23A-C28A-C30A	6(2)
C2-C1-C6-C5	1.0(4)	C24A-C23A-C28A-C27A	0.0(18)
C2-C1-C6-C7	176.9(2)	C24A-C23A-C28A-C30A	-175.6(12)
C1-C2-C3-C4	-0.4(4)	C23A-C24A-C25A-C26A	0.0(14)
C2-C3-C4-C5	0.4(4)	C24A-C25A-C26A-C27A	0.0(15)
C3-C4-C5-N1	-178.5(2)	C25A-C26A-C27A-C28A	0.0(17)

C3-C4-C5-C6	0.4(3)	C25A-C26A-C27A-C29A	178.1(15)
N1-C5-C6-C1	177.9(2)	C26A-C27A-C28A-C23A	-0.1(19)
N1-C5-C6-C7	2.2(3)	C26A-C27A-C28A-C30A	175.3(12)
C4-C5-C6-C1	-1.0(3)	C29A-C27A-C28A-C23A	-178.2(16)
C4-C5-C6-C7	-176.7(2)	C29A-C27A-C28A-C30A	-3(2)
C1-C6-C7-O1	23.7(3)	C1-C6-C7-O2	-154.9(2)
C5-C6-C7-O1	-160.6(2)		

Table S4. Bond distances for **3** (Å)

Co-O1	2.0556(8)	C2-C7	1.4928(14)
Co-O3A	2.1224(19)	C2-C3	1.4050(14)
Co-O4A	2.0803(14)	C3-C4	1.3842(13)
Co-O3B	2.069(3)	C4-C5	1.3959(14)
Co-O4B	2.134(3)	C5-C6	1.3824(14)
Co-O1_a	2.0556(8)	O5B-C18B	1.269(17)
Co-O3A_a	2.1224(19)	C8A-C13A	1.405(11)
Co-O4A_a	2.0803(14)	C8A-C9	1.350(10)
Co-O3B_a	2.069(3)	C8B-C9	1.450(9)
Co-O4B_a	2.134(3)	C8B-C13B	1.399(12)
O1-C7	1.2753(14)	C9-C10	1.3904(15)
O2-C7	1.2646(16)	C10-C11B	1.434(8)
O3A-C17A	1.427(5)	C10-C11A	1.329(10)
O3B-C17B	1.423(10)	C11A -C12A	1.376(11)
O4A-C16A	1.398(6)	C11B -C12B	1.408(9)
O4B-C16B	1.368(9)	C12A -C14A	1.514(7)
N1A-C8A	1.422(12)	C12A -C13A	1.398(8)
N1A-C1	1.360(5)	C12B -C13B	1.407(8)
N1B-C1	1.446(11)	C12B -C14B	1.513(7)
N1B-C8B	1.336(15)	C13A -C15A	1.511(7)
O3A-H3A	0.72(3)	C13B -C15B	1.516(7)
O3B-H3B	0.91(6)	C3-H3	0.9300
O4A-H4A	0.92(3)	C4-H4	0.9300
O4B-H4B	0.99(6)	C5-H5	0.9300
C1-C6	1.4136(13)	O5B-H5B	0.82(6)
C1-C2	1.4205(14)	C6-H6	0.9300
N1A-H1A	0.813(18)	C9-H9	1.000(16)
N1B-H1B	0.81(3)	C10-H10	0.926(16)
C11A -H11A	0.9300	C16B -H16F	0.9600
C11B -H11B	0.9300	C16B -H16E	0.9600
C14A -H14A	0.9600	C16B -H16D	0.9600
C14A -H14C	0.9600	C17A -H17B	0.9600
C14A -H14B	0.9600	C17A -H17A	0.9600
C14B -H14F	0.9600	C17A -H17C	0.9600
C14B -H14E	0.9600	C17B -H17F	0.9600
C14B -H14D	0.9600	C17B -H17D	0.9600
C15A -H15A	0.9600	C17B -H17E	0.9600
C15A -H15B	0.9600	O5A-C18A	1.465(9)

C15A -H15C	0.9600	O5A-H5A	0.8200
C15B -H15D	0.9600	C18B -H18C	0.9600
C15B -H15E	0.9600	C18B -H18A	0.9600
C15B -H15F	0.9600	C18B -H18B	0.9600
C16A -H16B	0.9600	C18A -H18D	0.9600
C16A -H16A	0.9600	C18A -H18E	0.9600
C16A -H16C	0.9600	C18A -H18F	0.9600

Table S5. Bond angles for **3**, (°)

O1-Co-O3A	88.44(5)	O3B_a-Co-O4B_a	91.47(16)
O1-Co-O4A	92.37(4)	Co-O1-C7	128.86(7)
O1-Co-O3B	90.01(9)	Co-O3A-C17A	130.1(2)
O1-Co-O4B	85.11(8)	Co-O3B-C17B	125.3(4)
O1-Co-O1_a	180.00	Co-O4A-C16A	127.4(3)
O1-Co-O3A_a	91.56(5)	Co-O4B-C16B	131.3(4)
O1-Co-O4A_a	87.63(4)	C1-N1A-C8A	120.5(6)
O1-Co-O3B_a	89.99(9)	C1-N1B-C8B	130.5(10)
O1-Co-O4B_a	94.89(8)	C17A-O3A-H3A	106(3)
O3A-Co-O4A	92.55(7)	Co-O3A-H3A	117(3)
O1_a-Co-O3A	91.56(5)	Co-O3B-H3B	115(4)
O3A-Co-O3A_a	180.00	C17B-O3B-H3B	107(4)
O3A-Co-O4A_a	87.45(7)	Co-O4A-H4A	100.9(17)
O1_a-Co-O4A	87.63(4)	C16A-O4A-H4A	108.4(15)
O3A_a-Co-O4A	87.45(7)	C16B-O4B-H4B	107(4)
O4A-Co-O4A_a	180.00	Co-O4B-H4B	103(4)
O3B-Co-O4B	91.47(16)	N1B-C1-C6	113.5(4)
O1_a-Co-O3B	89.99(9)	N1B-C1-C2	128.0(4)
O3B-Co-O3B_a	180.00	N1A-C1-C6	123.4(2)
O3B-Co-O4B_a	88.53(16)	C2-C1-C6	118.16(9)
O1_a-Co-O4B	94.89(8)	N1A-C1-C2	118.3(2)
O3B_a-Co-O4B	88.53(16)	C1-N1A-H1A	122.4(17)
O4B-Co-O4B_a	180.00	C1-N1B-H1B	109(4)
O1_a-Co-O3A_a	88.44(5)	C1-C2-C7	123.16(9)
O1_a-Co-O4A_a	92.37(4)	C3-C2-C7	117.81(9)
O1_a-Co-O3B_a	90.01(9)	C1-C2-C3	119.04(9)
O1_a-Co-O4B_a	85.11(8)	C2-C3-C4	121.96(9)
O3A_a-Co-O4A_a	92.55(7)	C3-C4-C5	118.90(9)
C4-C5-C6	120.65(9)	C4-C3-H3	119.00
C1-C6-C5	121.29(9)	C5-C4-H4	121.00
O2-C7-C2	118.96(10)	C3-C4-H4	121.00
O1-C7-C2	117.91(10)	C4-C5-H5	120.00
O1-C7-O2	123.13(10)	C6-C5-H5	120.00
N1A-C8A-C9	123.8(8)	C18B-O5B-H5B	114(5)
C9-C8A-C13A	117.6(8)	C5-C6-H6	119.00
C9-C8B-C13B	122.6(7)	C1-C6-H6	119.00
N1B-C8B-C9	116.7(9)	C8B-C9-H9	123.5(10)
C8B-C9-C10	115.5(4)	C8A-C9-H9	114.2(10)

C8A-C9-C10	124.7(5)	C10-C9-H9	121.0(9)
C9-C10-C11B	123.1(3)	C11A-C10-H10	123.2(10)
C9-C10-C11A	115.1(4)	C11B-C10-H10	114.9(10)
C10-C11A-C12A	124.7(8)	C9-C10-H10	121.8(10)
C10-C11B-C12B	118.9(6)	C12A-C11A-H11A	118.00
C13A-C12A-C14A	120.7(5)	C10-C11A-H11A	118.00
C11A-C12A-C13A	118.5(6)	C10-C11B-H11B	121.00
C11A-C12A-C14A	120.9(6)	C12B-C11B-H11B	121.00
C13B-C12B-C14B	120.7(5)	C12A-C14A-H14A	109.00
C11B-C12B-C14B	119.3(5)	C12A-C14A-H14B	110.00
C11B-C12B-C13B	120.0(6)	H14B-C14A-H14C	109.00
C12A-C13A-C15A	120.1(5)	H14A-C14A-H14B	109.00
C8A-C13A-C15A	121.4(6)	H14A-C14A-H14C	109.00
C8A-C13A-C12A	118.5(6)	C12A-C14A-H14C	109.00
C12B-C13B-C15B	120.5(5)	C12B-C14B-H14F	109.00
C8B-C13B-C15B	119.8(6)	H14D-C14B-H14E	109.00
C8B-C13B-C12B	119.5(6)	C12B-C14B-H14D	110.00
C2-C3-H3	119.00	C12B-C14B-H14E	109.00
H14E-C14B-H14F	109.00	H17B-C17A-H17C	110.00
H14D-C14B-H14F	109.00	O3A-C17A-H17A	109.00
C13A-C15A-H15C	109.00	O3A-C17A-H17B	109.00
C13A-C15A-H15B	109.00	H17A-C17A-H17B	110.00
H15A-C15A-H15C	109.00	H17A-C17A-H17C	109.00
H15B-C15A-H15C	109.00	O3A-C17A-H17C	109.00
C13A-C15A-H15A	109.00	O3B-C17B-H17E	109.00
H15A-C15A-H15B	109.00	O3B-C17B-H17F	109.00
H15D-C15B-H15F	109.00	O3B-C17B-H17D	109.00
H15E-C15B-H15F	109.00	H17D-C17B-H17F	109.00
H15D-C15B-H15E	109.00	H17E-C17B-H17F	110.00
C13B-C15B-H15D	109.00	H17D-C17B-H17E	110.00
C13B-C15B-H15E	109.00	C18A-O5A-H5A	109.00
C13B-C15B-H15F	109.00	O5B-C18B-H18B	109.00
O4A-C16A-H16A	110.00	O5B-C18B-H18C	109.00
O4A-C16A-H16C	110.00	O5B-C18B-H18A	110.00
H16A-C16A-H16B	109.00	H18A-C18B-H18C	110.00
H16A-C16A-H16C	109.00	H18B-C18B-H18C	109.00
H16B-C16A-H16C	109.00	H18A-C18B-H18B	110.00
O4A-C16A-H16B	109.00	O5A-C18A-H18D	109.00
O4B-C16B-H16E	109.00	O5A-C18A-H18E	109.00
O4B-C16B-H16F	110.00	O5A-C18A-H18F	109.00
H16D-C16B-H16F	110.00	H18D-C18A-H18E	109.00
H16E-C16B-H16F	109.00	H18D-C18A-H18F	109.00
O4B-C16B-H16D	109.00	H18E-C18A-H18F	110.00
H16D-C16B-H16E	109.00		

Table S6. Torsion angles for **3**, (°)

O3A-Co-O1-C7	109.18(11)	C1 -C2 -C3 -C4	-0.67(15)

O4A-Co -O1 -C7	16.69(11)	C7 -C2 -C3 -C4	179.53(10)
O3A_a-Co -O1 -C7	-70.82(11)	C1 -C2 -C7 -O1	-0.99(16)
O4A_a-Co -O1 -C7	-163.31(11)	C1 -C2 -C7 -O2	178.26(11)
O1 -Co -O3A-C17A	179.0(3)	C3 -C2 -C7 -O1	178.81(10)
O4A-Co -O3A-C17A	-88.7(3)	C3 -C2 -C7 -O2	-1.95(16)
O1_a-Co -O3A-C17A	-1.0(3)	C2 -C3 -C4 -C5	0.61(15)
O4A_a-Co -O3A-C17A	91.3(3)	C3 -C4 -C5 -C6	-0.25(15)
O1 -Co -O4A-C16A	117.9(3)	C4 -C5 -C6 -C1	-0.03(14)
O3A-Co -O4A-C16A	29.4(3)	N1A-C8A-C9 -C10	179.9(7)
O1_a-Co -O4A-C16A	-62.1(3)	C13A-C8A-C9 -C10	-10.1(14)
O3A_a-Co -O4A-C16A	-150.6(3)	N1A-C8A-C13A-C12A	-179.1(8)
Co -O1 -C7 -C2	164.91(7)	N1A-C8A-C13A-C15A	-1.1(15)
Co -O1 -C7 -O2	-14.30(18)	C9 -C8A-C13A-C12A	10.3(14)
C8A-N1A-C1 -C6	2.1(7)	C9 -C8A-C13A-C15A	-171.7(8)
C8A-N1A-C1 -C2	178.0(5)	C8A-C9 -C10-C11A	2.2(9)
C1 -N1A-C8A-C9	-113.3(10)	C9 -C10-C11A-C12A	5.7(12)
C1 -N1A-C8A-C13A	76.7(11)	C10-C11A-C12A-C13A	-5.0(15)
N1A-C1 -C6 -C5	175.9(3)	C10-C11A-C12A-C14A	175.8(8)
C2 -C1 -C6 -C5	-0.03(14)	C11A-C12A-C13A-C8A	-3.3(13)
N1A-C1 -C2 -C7	4.0(3)	C11A-C12A-C13A-C15A	178.6(8)
C6 -C1 -C2 -C3	0.37(15)	C14A-C12A-C13A-C8A	175.8(9)
N1A-C1 -C2 -C3	-175.8(2)	C14A-C12A-C13A-C15A	-2.2(11)
C6 -C1 -C2 -C7	-179.84(10)		

Table S7. Bond distances for **4** (Å)

Ni-O1	2.0208(8)	N2B -H2B	0.83(3)
Ni-O3A	2.0504(16)	C3-C4	1.3962(14)
Ni-O4A	2.088(2)	C4-C5	1.3846(13)
Ni-O3B	2.112(3)	C5-C6	1.4047(14)
Ni-O4B	2.051(2)	O5A-C18A	1.482(6)
Ni-O1_a	2.0208(8)	C6-C7	1.4913(14)
Ni-O3A_a	2.0504(16)	C8A-C9A	1.390(7)
Ni-O4A_a	2.088(2)	C8A-C13A	1.390(6)
Ni-O3B_a	2.112(3)	C8B-C13B	1.390(5)
Ni-O4B_a	2.051(2)	C8B-C10B	1.390(6)
O1-C7	1.2780(14)	C9A-C10A	1.390(7)
O2-C7	1.2625(17)	C9B-C10B	1.391(6)
O3A-C17A	1.415(16)	C9B-C11B	1.390(6)
O3B-C17B	1.40(3)	C10A-C11A	1.389(7)
O4A-C16A	1.441(5)	C11A-C12A	1.390(5)
O4B-C16B	1.385(7)	C11B-C12B	1.390(5)
N2A-C1	1.384(8)	C12A-C14A	1.526(5)
N2A-C8A	1.404(9)	C12A-C13A	1.390(5)
N2B-C1	1.398(7)	C12B-C14B	1.518(5)
N2B-C8B	1.429(8)	C12B-C13B	1.390(5)
O3A-H3A	0.84(2)	C13A-C15A	1.527(4)
O3B-H3B	0.86(3)	C13B-C15B	1.533(4)

O4A-H4A	0.84(3)	C2-H2	0.9300
O4B-H4B	0.84(4)	C3-H3	0.9300
C1-C6	1.4211(14)	C4-H4	0.9300
C1-C2	1.4126(13)	C5-H5	0.9300
C2-C3	1.3844(14)	O5A-H5A	0.83(7)
N2A-H2A	0.80(3)	C9A-H9A	0.9300
C9B-H9B	0.9300	C16A-H16D	0.9600
C10A-H10A	0.9300	C16B-H16B	0.9600
C10B-H10B	0.9300	C16B-H16A	0.9600
C11A-H11A	0.9300	C16B-H16C	0.9600
C11B-H11B	0.9300	C17A-H17F	0.9600
C14A-H14C	0.9600	C17A-H17D	0.9600
C14A-H14B	0.9600	C17A-H17E	0.9600
C14A-H14A	0.9600	C17B-H17C	0.9600
C14B-H14F	0.9600	C17B-H17A	0.9600
C14B-H14E	0.9600	C17B-H17B	0.9600
C14B-H14D	0.9600	O5B-C18B	1.309(7)
C15A-H15A	0.9600	O5B-H5B	0.83(6)
C15A-H15C	0.9600	C18A-H18F	0.9600
C15A-H15B	0.9600	C18A-H18D	0.9600
C15B-H15D	0.9600	C18A-H18E	0.9600
C15B-H15E	0.9600	C18B-H18A	0.9600
C15B-H15F	0.9600	C18B-H18B	0.9600
C16A-H16E	0.9600	C18B-H18C	0.9600
C16A-H16F	0.9600		

Table S8. Bond angles for **4**, (°)

O3A-Ni-O4A_a	92.40(7)	Ni-O4A-H4A	114(2)
O1_a-Ni-O4A	92.90(5)	C16A-O4A-H4A	104(2)
O3A_a-Ni-O4A	92.40(7)	C16B-O4B-H4B	114(4)
O4A-Ni-O4A_a	180.00	Ni-O4B-H4B	107(4)
O3B-Ni-O4B	89.55(14)	N2B-C1-C2	124.7(3)
O1_a-Ni-O3B	85.95(7)	N2B-C1-C6	116.9(3)
O3B-Ni-O3B_a	180.00	N2A-C1-C6	127.4(3)
O3B-Ni-O4B_a	90.45(14)	N2A-C1-C2	114.1(3)
O1_a-Ni-O4B	89.64(8)	C2-C1-C6	118.20(9)
O3B_a-Ni-O4B	90.45(14)	C1-C2-C3	121.27(9)
O4B-Ni-O4B_a	180.00	C8A-N2A-H2A	120(4)
O1_a-Ni-O3A_a	86.19(5)	C1-N2A-H2A	108(4)
O1_a-Ni-O4A_a	87.10(5)	C8B-N2B-H2B	119(3)
O1_a-Ni-O3B_a	94.05(7)	C1-N2B-H2B	120(3)
O1_a-Ni-O4B_a	90.36(8)	C2-C3-C4	120.64(9)
O3A_a-Ni-O4A_a	87.60(7)	C3-C4-C5	118.85(9)
C4-C5-C6	122.04(9)	C8B-C13B-C12B	120.0(3)
C5-C6-C7	117.77(9)	C8B-C13B-C15B	120.3(3)
C1-C6-C5	119.01(8)	C12B-C13B-C15B	119.4(3)
C1-C6-C7	123.22(9)	C3-C2-H2	119.00

O1-C7-C6	117.91(10)	C1-C2-H2	119.00
O2-C7-C6	118.89(10)	C4-C3-H3	120.00
O1-C7-O2	123.20(10)	C2-C3-H3	120.00
C9A-C8A-C13A	120.0(4)	C3-C4-H4	121.00
N2A-C8A-C9A	117.5(5)	C5-C4-H4	121.00
N2A-C8A-C13A	122.5(5)	C4-C5-H5	119.00
N2B-C8B-C10B	119.5(4)	C6-C5-H5	119.00
N2B-C8B-C13B	120.4(4)	C18A-O5A-H5A	123(10)
C10B-C8B-C13B	120.0(4)	C8A-C9A-H9A	120.00
C8A-C9A-C10A	120.0(5)	C10A-C9A-H9A	120.00
C10B-C9B-C11B	120.0(3)	C10B-C9B-H9B	120.00
C9A-C10A-C11A	120.0(4)	C11B-C9B-H9B	120.00
C8B-C10B-C9B	120.0(4)	C9A-C10A-H10A	120.00
C10A-C11A-C12A	120.0(4)	C11A-C10A-H10A	120.00
C9B-C11B-C12B	120.0(3)	C8B-C10B-H10B	120.00
C11A-C12A-C13A	120.0(3)	C9B-C10B-H10B	120.00
C13A-C12A-C14A	121.0(3)	C12A-C11A-H11A	120.00
C11A-C12A-C14A	119.0(3)	C10A-C11A-H11A	120.00
C13B-C12B-C14B	121.2(3)	C12B-C11B-H11B	120.00
C11B-C12B-C14B	118.8(3)	C9B-C11B-H11B	120.00
C11B-C12B-C13B	120.0(3)	C12A-C14A-H14A	109.00
C12A-C13A-C15A	120.4(3)	C12A-C14A-H14C	109.00
C8A-C13A-C12A	120.0(3)	H14A-C14A-H14B	109.00
C8A-C13A-C15A	119.5(3)	C12A-C14A-H14B	109.00
H14B-C14A-H14C	109.00	H16B-C16B-H16C	109.00
H14A-C14A-H14C	110.00	H16A-C16B-H16C	109.00
H14E-C14B-H14F	109.00	O4B-C16B-H16C	109.00
C12B-C14B-H14F	109.00	H16A-C16B-H16B	109.00
C12B-C14B-H14E	109.00	H17E-C17A-H17F	109.00
C12B-C14B-H14D	109.00	H17D-C17A-H17E	109.00
H14D-C14B-H14F	110.00	H17D-C17A-H17F	109.00
H14D-C14B-H14E	109.00	O3A-C17A-H17E	109.00
C13A-C15A-H15B	109.00	O3A-C17A-H17F	110.00
C13A-C15A-H15A	109.00	O3A-C17A-H17D	110.00
H15A-C15A-H15B	109.00	O3B-C17B-H17B	109.00
C13A-C15A-H15C	109.00	O3B-C17B-H17C	110.00
H15A-C15A-H15C	109.00	O3B-C17B-H17A	110.00
H15B-C15A-H15C	109.00	H17A-C17B-H17C	110.00
C13B-C15B-H15E	109.00	H17B-C17B-H17C	109.00
C13B-C15B-H15D	109.00	H17A-C17B-H17B	109.00
C13B-C15B-H15F	109.00	C18B-O5B-H5B	95(5)
H15D-C15B-H15E	110.00	O5A-C18A-H18E	109.00
H15E-C15B-H15F	110.00	O5A-C18A-H18F	109.00
H15D-C15B-H15F	109.00	O5A-C18A-H18D	109.00
H16D-C16A-H16E	109.00	H18D-C18A-H18F	109.00
H16D-C16A-H16F	110.00	H18E-C18A-H18F	109.00
O4A-C16A-H16F	109.00	H18D-C18A-H18E	109.00
O4A-C16A-H16D	109.00	O5B-C18B-H18A	109.00

H16E-C16A-H16F	109.00	O5B-C18B-H18B	109.00
O4A-C16A-H16E	109.00	O5B-C18B-H18C	110.00
O4B-C16B-H16A	109.00	H18A-C18B-H18B	109.00
O4B-C16B-H16B	109.00	H18A-C18B-H18C	109.00
H18B-C18B-H18C	109.00		

Table S9. Torsion angles for **4**, (°)

O3A-Ni-O1-C7	-165.91(11)	N2B-C1-C6-C7	5.9(3)
O4A-Ni-O1-C7	106.31(12)	C1-C2-C3-C4	-0.05(17)
O3A_a-Ni-O1-C7	14.09(11)	C2-C3-C4-C5	-0.12(14)
O4A_a-Ni-O1-C7	-73.69(12)	C3-C4-C5-C6	0.46(15)
O1-Ni-O3A-C17A	66.9(9)	C4-C5-C6-C1	-0.61(15)
O4A-Ni-O3A-C17A	154.2(9)	C4-C5-C6-C7	179.05(10)
O1_a-Ni-O3A-C17A	-113.1(9)	C1-C6-C7-O2	178.49(11)
O4A_a-Ni-O3A-C17A	-25.8(9)	C5-C6-C7-O1	179.42(10)
O1-Ni-O4A-C16A	176.9(3)	C5-C6-C7-O2	-1.16(17)
O3A-Ni-O4A-C16A	90.5(3)	C1-C6-C7-O1	-0.94(16)
O1_a-Ni-O4A-C16A	-3.2(3)	N2B-C8B-C10B-C9B	178.1(5)
O3A_a-Ni-O4A-C16A	-89.5(3)	C13B-C8B-C10B-C9B	0.0(8)
Ni-O1-C7-C6	166.37(8)	N2B-C8B-C13B-C12B	-178.1(5)
Ni-O1-C7-O2	-13.03(19)	N2B-C8B-C13B-C15B	8.0(7)
C8B-N2B-C1-C6	-178.9(4)	C10B-C8B-C13B-C12B	0.0(7)
C8B-N2B-C1-C2	6.6(7)	C10B-C8B-C13B-C15B	-173.9(5)
C1-N2B-C8B-C10B	-110.5(6)	C11B-C9B-C10B-C8B	0.0(8)
C1-N2B-C8B-C13B	67.7(7)	C10B-C9B-C11B-C12B	0.0(8)
C2-C1-C6-C5	0.42(14)	C9B-C11B-C12B-C13B	-0.1(8)
C2-C1-C6-C7	-179.22(10)	C9B-C11B-C12B-C14B	179.1(5)
C6-C1-C2-C3	-0.10(15)	C11B-C12B-C13B-C8B	0.1(7)
N2B-C1-C6-C5	-174.5(3)	C11B-C12B-C13B-C15B	174.0(5)
N2B-C1-C2-C3	174.4(3)	C14B-C12B-C13B-C8B	-179.1(5)
		C14B-C12B-C13B-C15B	-5.1(8)