Electronic Supplementary Material (ESI) for CrystEngComm

Title: Host-guest chemistry of Ni^{II} coordination compounds with PDC and $(py)_2CO$: reversible crystal-to-amorphous transformations induced by solvent exchange

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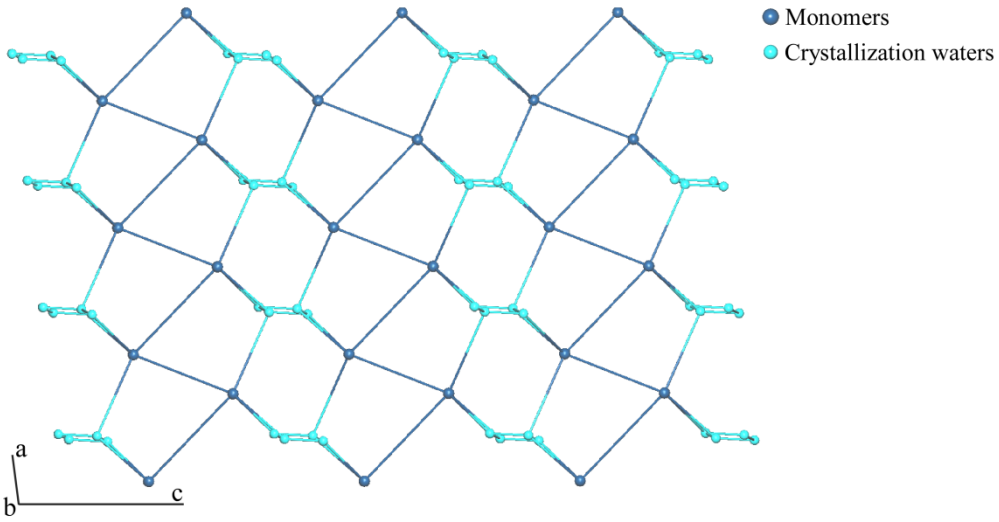

Figure S1.- Simplification of the topology for compound **1a** where the zig-zag fashion adopted by the monomers can be observed.

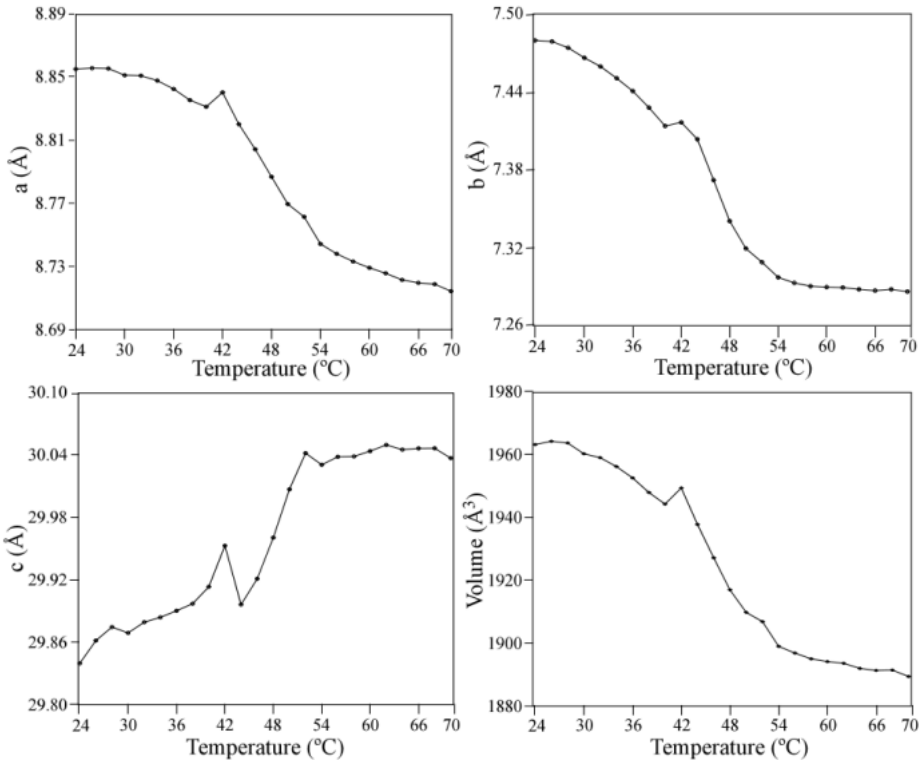

Figure S2.- Cyclic refinement of the cell parameters for compound **1a**.

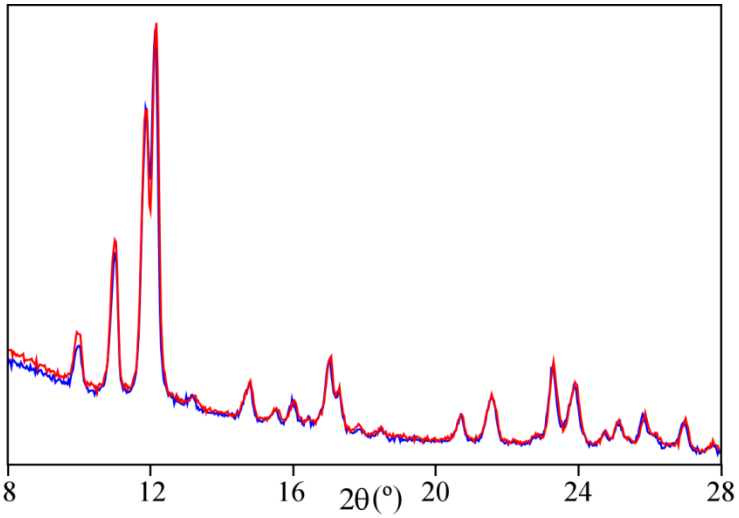

Figure S3.- Comparison of the diffractograms for compounds **1a** (blue) and **1b** after rehydration (red).

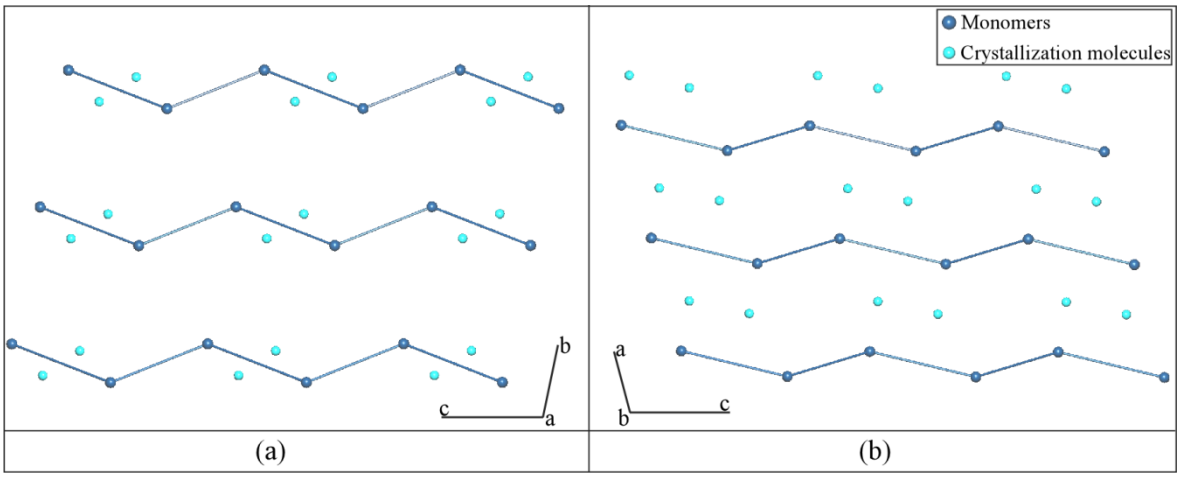

Figure S4.- Simplification of the topologies for compounds **3m** (a) and **3p** (b) where the zig-zag fashion adopted by the monomers can be observed.

Table S1.- Hydrogen bonds (Å, Deg.) calculated by PLATON software for compound **1a**.

Donor --- H....Acceptor	D – H	H....A	D....A	D - H....A
O(1W)---H(1A)….O(3W)	0.82(2)	1.81(2)	2.629(3)	174(3)
O(1W)---H(1B)….O(4)	0.82(2)	1.88(2)	2.695(3)	176(3)
O(2W)---H(2A)….O(1)	0.83(3)	2.00(2)	2.814(3)	170(3)
O(2W)---H(2B)….O(6)	0.84(2)	2.04(3)	2.858(3)	167(3)
O(3W)---H(3A)….O(2W)	0.838(19)	1.933(17)	2.739(3)	161(3)
O(3W)---H(3B)….O(2W)	0.833(17)	2.478(19)	3.167(3)	141(3)
O(3W)---H(3B)….O(2)	0.833(17)	2.21(3)	2.809 (3)	129(2)
O(5)---H(5H)….O(3)	0.832(17)	1.825(18)	2.650(2)	171(2)
O(6)---H(6H)….O(4)	0.84(2)	1.76(2)	2.592(2)	173(3)

Table S2.- Analysis of short ring-interactions with Cg-Cg Distances < 4.0 Å and Beta < 60.0 Deg. calculated by PLATON software for compound **1a**. The Cg(5) ring corresponds to the PDC ligand and the Cg(6) ring to the dpk ligand. Alpha: Dihedral Angle between Planes I and J (Deg); Beta: Angle Cg(I)--Cg(J) or Cg(I)--Me vector and normal to plane I (Deg); Gamma: Angle Cg(I)--Cg(J) vector and normal to plane J (Deg).

Cg(I)·····Cg(J)	D(Cg-Cg)	Alpha	Beta	Gamma
Cg(5)·····Cg(5)	3.8029(14)	0	23.43	23.43
Cg(6)·····Cg(6)	3.8176(15)	14	11.27	18.74

Table S3.- Hydrogen bonds (Å, Deg.) calculated by PLATON software for compound **3m**.

Donor --- H....Acceptor	D – H	H....A	D....A	D - H....A
O(5)---H(5H)....O(3)	0.83(9)	1.79(7)	2.593(6)	163(17)
O(6)---H(6H)....O(4)	0.86(7)	1.78(6)	2.630(7)	173(11)
O(7)---H(7H)....O(2)	0.84(7)	1.79(4)	2.615(6)	169(19)

Table S4.- Analysis of short ring-interactions with Cg-Cg Distances < 4.0 Å and Beta < 60.0 Deg. calculated by PLATON software for compound **3m**. The Cg(7) ring corresponds to the dpk ligand. Alpha: Dihedral Angle between Planes I and J (Deg); Beta: Angle Cg(I)--Cg(J) or Cg(I)--Me vector and normal to plane I (Deg); Gamma: Angle Cg(I)--Cg(J) vector and normal to plane J (Deg).

Cg(I)·····Cg(J)	D(Cg-Cg)	Alpha	Beta	Gamma
Cg(7)·····Cg(7)	3.764(3)	0	17.10	17.10

Table S5.- Hydrogen bonds (Å, Deg.) calculated by PLATON software for compound **3p**.

Donor --- H....Acceptor	D – H	H....A	D....A	D - H....A
O(5)---H(5H)....O(3)	0.83(8)	1.75(8)	2.572(4)	174(10)
O(6)---H(6H)....O(4)	0.83(5)	1.77(5)	2.599(6)	179(12)
O(7)---H(7H)....O(2)	0.81(2)	1.83(3)	2.635(4)	169(9)

Table S6.- Analysis of short ring-interactions with Cg-Cg Distances < 4.0 Å and Beta < 60.0 Deg. calculated by PLATON software for compound **3p**. The Cg(6) ring corresponds to the dpk ligand. Alpha: Dihedral Angle between Planes I and J (Deg); Beta: Angle Cg(I)--Cg(J) or Cg(I)--Me vector and normal to plane I (Deg); Gamma: Angle Cg(I)--Cg(J) vector and normal to plane J (Deg).

Cg(I)·····Cg(J)	D(Cg-Cg)	Alpha	Beta	Gamma
Cg(6)·····Cg(6)	3.499(3)	0	20.3	20.3

Table S7.- Hydrogen bonds (Å, Deg.) calculated by PLATON software for compound **3e**.

Donor....Acceptor	D....A
O(3)....O(5)	2.300
O(4)....O(6)	2.640

Table S8.- Analysis of short ring-interactions with Cg-Cg Distances < 4.0 Å and Beta < 60.0 Deg. calculated by PLATON software for compound **3e**. The Cg(6) ring corresponds to the dpk ligand. Alpha: Dihedral Angle between Planes I and J (Deg); Beta: Angle Cg(I)--Cg(J) or Cg(I)--Me vector and normal to plane I (Deg); Gamma: Angle Cg(I)--Cg(J) vector and normal to plane J (Deg).

Cg(I)·····Cg(J)	D(Cg-Cg)	Alpha	Beta	Gamma
Cg(6)·····Cg(6)	3.6728	0	27.35	27.35

Table S9.- Fractional atomic coordinates and isotropic (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **1a**.

Atom	X	y	z	U(eq) [$Å^2$]
Ni1	2034(1)	408(1)	3691(1)	17(1)
O1	3283(2)	-1749(3)	3524(1)	23(1)
O1W	3898(2)	2051(3)	3745(1)	24(1)
O2	4995(2)	-3757(3)	3827(1)	35(1)
O2W	4881(2)	1931(3)	7185(1)	38(1)
O3	1289(2)	659(2)	5576(1)	21(1)
O3W	4691(3)	1034(3)	8068(1)	49(1)
O4	3527(2)	-330(3)	5919(1)	24(1)
O5	-210(2)	-763(2)	3632(1)	18(1)
O6	-2573(2)	280(3)	3292(1)	22(1)
N1	2686(2)	-641(3)	4330(1)	17(1)
N2	1211(2)	885(3)	3024(1)	19(1)
N3	703(2)	2541(3)	3867(1)	18(1)
C1	3703(3)	-1990(3)	4319(1)	19(1)
C2	4396(3)	-2800(3)	4709(1)	21(1)
C3	4045(3)	-2192(4)	5124(1)	21(1)
C4	2977(3)	-818(3)	5136(1)	17(1)
C5	2309(3)	-87(3)	4729(1)	16(1)
C6	4045(3)	-2569(4)	3855(1)	24(1)
C7	2549(3)	-97(3)	5577(1)	18(1)
C8	1980(3)	1063(3)	2666(1)	21(1)
C9	1246(3)	1267(4)	2232(1)	23(1)
C10	-332(3)	1290(4)	2166(1)	24(1)
C11	-1137(3)	1104(4)	2536(1)	22(1)
C12	-321(3)	895(3)	2957(1)	18(1)
C13	-1044(3)	679(3)	3391(1)	18(1)
C14	-753(3)	2398(3)	3678(1)	17(1)
C15	-1841(3)	3686(4)	3735(1)	21(1)
C16	-1418(3)	5151(4)	4009(1)	24(1)
C17	79(3)	5307(4)	4208(1)	25(1)
C18	1112(3)	3981(4)	4123(1)	22(1)

Table S10.- Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **1a**.

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	13(1)	24(1)	15(1)	0(1)	1(1)	3(1)
O1	20(1)	31(1)	18(1)	-3(1)	1(1)	7(1)
O1W	14(1)	33(1)	26(1)	4(1)	0(1)	2(1)
O2	36(1)	40(1)	27(1)	-8(1)	0(1)	21(1)
O2W	27(1)	56(2)	31(1)	-12(1)	7(1)	-3(1)
O3	19(1)	25(1)	19(1)	0(1)	3(1)	5(1)
O3W	76(2)	37(1)	31(1)	2(1)	2(1)	13(1)
O4	16(1)	38(1)	16(1)	1(1)	0(1)	3(1)
O5	18(1)	21(1)	15(1)	1(1)	2(1)	4(1)
O6	15(1)	32(1)	19(1)	-1(1)	2(1)	-1(1)
N1	14(1)	21(1)	16(1)	1(1)	1(1)	2(1)
N2	18(1)	23(1)	16(1)	0(1)	1(1)	3(1)
N3	15(1)	21(1)	17(1)	1(1)	2(1)	3(1)
C1	14(1)	22(1)	22(1)	-3(1)	2(1)	2(1)
C2	17(1)	20(1)	25(1)	0(1)	0(1)	6(1)
C3	17(1)	26(1)	20(1)	4(1)	0(1)	2(1)
C4	12(1)	21(1)	18(1)	1(1)	2(1)	-1(1)
C5	13(1)	18(1)	18(1)	-1(1)	2(1)	2(1)
C6	20(1)	29(1)	21(1)	-5(1)	1(1)	4(1)

C7	16(1)	19(1)	18(1)	1(1)	2(1)	-2(1)
C8	19(1)	24(1)	22(1)	-1(1)	5(1)	0(1)
C9	27(1)	24(1)	18(1)	0(1)	6(1)	0(1)
C10	28(1)	25(1)	17(1)	2(1)	-1(1)	-1(1)
C11	19(1)	24(1)	22(1)	1(1)	0(1)	0(1)
C12	18(1)	18(1)	19(1)	0(1)	2(1)	0(1)
C13	14(1)	22(1)	17(1)	1(1)	0(1)	3(1)
C14	16(1)	21(1)	16(1)	3(1)	3(1)	-1(1)
C15	15(1)	24(1)	24(1)	4(1)	2(1)	1(1)
C16	23(1)	20(1)	30(1)	2(1)	7(1)	7(1)
C17	26(1)	23(1)	27(1)	-3(1)	3(1)	-1(1)
C18	20(1)	23(1)	22(1)	0(1)	-2(1)	-2(1)

Table S11.- Geometric parameters (Å, º) for compound **1a**.

N1-Ni1	2.072(2)	C7-O4	1.267(3)
N2-Ni1	2.065(2)	C8-N2	1.338(3)
N3-Ni1	2.074(2)	C8-C9	1.386(3)
Ni1-O1	2.0383(18)	C9-C10	1.384(4)
Ni1-O1W	2.0387(19)	C10-C11	1.390(4)
Ni1-O5	2.1510(17)	C11-C12	1.378(3)
C1-N1	1.347(3)	C12-N2	1.343(3)
C1-C2	1.384(3)	C12-C13	1.520(3)
C1-C6	1.514(3)	C13-O6	1.379(3)
C2-C3	1.384(4)	C13-O5	1.440(3)
C3-C4	1.392(3)	C13-C14	1.540(3)
C4-C5	1.394(3)	C14-N3	1.344(3)
C4-C7	1.508(3)	C14-C15	1.379(3)
C5-N1	1.339(3)	C15-C16	1.383(4)
C6-O2	1.226(3)	C16-C17	1.387(4)
C6-O1	1.280(3)	C17-C18	1.385(4)
C7-O3	1.245(3)	C18-N3	1.337(3)

N1-C1-C2	122.2(2)	C8-N2-C12	118.6(2)
N1-C1-C6	115.9(2)	C8-N2-Ni1	129.13(17)
N1-C5-C4	122.1(2)	C12-N2-Ni1	112.18(16)
O2-C6-O1	126.1(2)	C18-N3-C14	118.8(2)
O2-C6-C1	118.6(2)	C18-N3-Ni1	129.06(17)
O1-C6-C1	115.3(2)	C14-N3-Ni1	112.12(16)
O3-C7-O4	126.0(2)	O1-Ni1-O1W	91.84(8)
O3-C7-C4	118.2(2)	O1-Ni1-N2	92.10(8)
O4-C7-C4	115.8(2)	O1W-Ni1-N2	99.26(8)
N2-C8-C9	122.0(2)	O1-Ni1-N1	80.31(7)
N2-C12-C11	123.0(2)	O1W-Ni1-N1	91.09(8)
N2-C12-C13	112.9(2)	N2-Ni1-N1	167.39(9)
O6-C13-O5	112.2(2)	O1-Ni1-N3	178.03(8)
O6-C13-C12	109.78(19)	O1W-Ni1-N3	90.05(8)
O5-C13-C12	105.16(18)	N2-Ni1-N3	88.13(8)
O6-C13-C14	113.07(19)	N1-Ni1-N3	99.11(8)
O5-C13-C14	107.24(18)	O1-Ni1-O5	100.58(7)
N3-C14-C15	122.6(2)	O1W-Ni1-O5	167.10(7)
N3-C14-C13	112.7(2)	N2-Ni1-O5	76.99(7)
N3-C18-C17	122.1(2)	N1-Ni1-O5	94.40(7)
C5-N1-C1	119.0(2)	N3-Ni1-O5	77.56(7)
C5-N1-Ni1	129.07(16)	C6-O1-Ni1	115.69(16)
C1-N1-Ni1	111.78(15)	C13-O5-Ni1	98.78(13)

Table S12.- Fractional atomic coordinates and isotropic (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **3m**.

Atom	x	y	z	U(eq) [$Å^2$]
Ni1	395(1)	1548(1)	3268(1)	33(1)
O1	-1273(6)	775(4)	4103(3)	45(1)
O2	-3275(5)	-1214(4)	4222(3)	47(1)
O3	-1673(6)	-1771(3)	-661(3)	50(1)
O4	-2948(6)	-3920(3)	-478(3)	50(1)
O5	2287(5)	2649(3)	2536(3)	37(1)
O6	3245(7)	4935(4)	2327(4)	69(2)
O7	2147(7)	656(5)	3870(3)	58(1)
O8	3450(20)	-347(15)	952(12)	258(6)
N1	-1168(6)	-309(4)	2313(3)	34(1)
N2	-967(6)	2611(4)	2510(3)	38(1)
N3	1715(6)	3422(4)	4237(3)	36(1)
C1	-2342(4)	-1118(2)	2746(2)	35(1)
C2	-3540(8)	-2404(5)	2267(4)	39(1)
C3	-3518(4)	-2932(2)	1323(2)	38(1)
C4	-2338(7)	-2122(4)	859(4)	30(1)
C5	-1206(7)	-799(5)	1381(4)	32(1)
C6	-2314(7)	-474(5)	3766(4)	34(1)
C7	-2310(7)	-2647(5)	-174(4)	34(1)
C8	-2737(9)	2290(7)	2183(5)	56(2)
C9	-3438(12)	3028(9)	1620(6)	75(2)
C10	-2315(14)	4132(8)	1348(6)	84(3)
C11	-491(6)	4499(4)	1674(3)	66(2)
C12	124(9)	3711(5)	2252(4)	45(2)
C13	2077(8)	3965(5)	2695(4)	40(2)
C14	2437(4)	4440(2)	3800(2)	41(2)
C15	3313(4)	5792(2)	4293(2)	66(2)
C16	1837(6)	3721(4)	5202(3)	51(2)
C17	2702(6)	5051(4)	5754(3)	67(2)
C18	3479(4)	6097(2)	5300(2)	78(3)
C19	2654(15)	-395(11)	3496(7)	121(4)
C30	2740(20)	-1597(16)	636(12)	169(6)

Table S13.- Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **3m**.

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	37(1)	28(1)	22(1)	2(1)	9(1)	-3(1)
O1	54(3)	38(2)	29(2)	0(2)	17(2)	-4(2)
O2	46(3)	49(2)	29(2)	10(2)	16(2)	-7(2)
O3	68(3)	35(2)	28(2)	5(2)	19(2)	-9(2)
O4	74(3)	31(2)	34(2)	1(2)	22(2)	0(2)
O5	38(2)	36(2)	27(2)	4(2)	11(2)	0(2)
O6	76(4)	48(2)	51(3)	5(2)	26(3)	-20(2)
O7	91(4)	64(3)	28(3)	5(2)	9(2)	43(3)
N1	36(3)	30(2)	25(3)	9(2)	10(2)	-5(2)
N2	38(3)	35(2)	28(3)	0(2)	8(2)	-2(2)
N3	34(3)	37(2)	20(2)	-5(2)	3(2)	-2(2)
C1	38(3)	33(2)	23(3)	6(2)	9(2)	-2(2)
C2	43(3)	29(2)	34(3)	2(2)	18(3)	-6(2)
C3	46(4)	24(2)	30(3)	-2(2)	11(3)	-4(2)
C4	33(3)	25(2)	27(3)	3(2)	10(2)	4(2)
C5	32(3)	34(2)	23(3)	8(2)	12(2)	-2(2)
C6	38(3)	36(3)	24(3)	8(2)	9(2)	6(2)
C7	35(3)	32(3)	27(3)	3(2)	7(2)	3(2)

C8	49(4)	64(4)	48(4)	5(3)	9(3)	16(3)
C9	59(5)	89(5)	67(6)	2(5)	-4(4)	30(5)
C10	121(8)	84(5)	51(5)	2(4)	-5(5)	59(6)
C11	105(7)	46(3)	45(5)	15(3)	19(4)	21(4)
C12	69(4)	30(2)	27(3)	2(2)	15(3)	7(3)
C13	49(4)	28(2)	26(3)	1(2)	14(3)	-9(2)
C14	43(3)	31(2)	35(3)	-4(2)	15(3)	-3(2)
C15	76(5)	44(3)	47(4)	-5(3)	22(4)	-15(3)
C16	61(4)	47(3)	30(4)	-2(3)	12(3)	3(3)
C17	93(6)	58(4)	27(4)	-15(3)	11(4)	7(4)
C18	97(6)	42(3)	53(5)	-22(3)	19(4)	-16(4)
C19	156(10)	181(10)	46(6)	-28(6)	-23(6)	127(9)

Table S14.- Geometric parameters (Å, º) for compound **3m**.

Ni1-N1	2.080(4)	N3-C16	1.338(5)
Ni1-N2	2.098(5)	N3-C14	1.324(4)
Ni1-N3	2.072(4)	C1-C2	1.377(6)
Ni1-O1	1.999(3)	C1-C6	1.505(6)
Ni1-O5	2.121(3)	C3-C2	1.384(6)
Ni1-O7	2.094(5)	C4-C3	1.381(5)
O1-C6	1.276(6)	C4-C5	1.406(7)
O2-C6	1.242(5)	C4-C7	1.500(7)
O3-C7	1.251(5)	C8-C9	1.370(11)
O4-C7	1.248(6)	C11-C10	1.392(11)
O5-C13	1.448(7)	C12-C11	1.389(8)
O6-C13	1.374(5)	C12-C13	1.538(10)
O7-C19	1.385(10)	C14-C13	1.522(6)
O8-C30	1.230(17)	C14-C15	1.3823
N1-C1	1.349(4)	C15-C18	1.3900
N1-C5	1.343(6)	C17-C16	1.3900
N2-C12	1.343(6)	C18-C17	1.375(4)
N2-C8	1.358(8)		

O1-Ni1-N3	94.53(15)	C12-N2-Ni1	112.8(4)
O1-Ni1-N1	81.60(15)	C8-N2-Ni1	130.0(4)
N3-Ni1-N1	174.21(17)	N1-C5-C4	123.4(4)
O1-Ni1-O7	91.45(19)	N3-C14-C15	123.2(2)
N3-Ni1-O7	93.9(2)	N3-C14-C13	112.3(3)
N1-Ni1-O7	90.53(19)	N1-C1-C2	122.2(3)
O1-Ni1-N2	100.18(18)	N1-C1-C6	114.9(3)
N3-Ni1-N2	84.67(18)	O4-C7-O3	125.6(5)
N1-Ni1-N2	91.76(18)	O4-C7-C4	117.2(4)
O7-Ni1-N2	168.35(17)	O3-C7-C4	117.2(4)
O1-Ni1-O5	171.45(14)	N2-C8-C9	123.5(6)
N3-Ni1-O5	77.00(15)	N2-C12-C11	122.7(6)
N1-Ni1-O5	106.77(14)	N2-C12-C13	111.0(5)
O7-Ni1-O5	90.28(18)	C11-C12-C13	126.3(4)
N2-Ni1-O5	78.13(16)	O6-C13-O5	112.3(5)
C13-O5-Ni1	99.5(3)	O6-C13-C14	109.2(4)
C6-O1-Ni1	114.5(3)	O5-C13-C14	106.5(4)
C19-O7-Ni1	133.4(5)	O6-C13-C12	113.0(5)
C14-N3-C16	118.3(4)	O5-C13-C12	107.4(4)
C14-N3-Ni1	113.0(3)	C14-C13-C12	108.1(4)
C16-N3-Ni1	128.6(3)	O2-C6-O1	125.2(5)
C5-N1-C1	117.5(4)	O2-C6-C1	117.2(4)
C5-N1-Ni1	131.7(3)	O1-C6-C1	117.6(3)
C1-N1-Ni1	110.8(3)	N3-C16-C17	122.3(2)

C12-N2-C8	117.0(5)		

Table S15.- Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for compound **3e**.

Atom	x	y	z	U(eq) [$Å^2$]
Ni1	0.126(7)	0.407(5)	0.189(3)	0.0264
O1	0.210(17)	0.549(11)	0.136(11)	0.0264
O2	0.128(17)	0.726(14)	0.115(10)	0.0264
O3	-0.03(2)	0.688(11)	0.592(8)	0.0264
O4	-0.03(2)	0.873(8)	0.556(7)	0.0264
O5	0.07(2)	0.256(12)	0.250(14)	0.0264
O6	0.131(13)	0.064(11)	0.275(11)	0.0264
O7a	-0.128(9)	0.339(8)	0.143(6)	0.0348
O8a	0.672303	0.937429	0.336788	0.06
N1a	0.073(5)	0.564(6)	0.292(4)	0.0245
N2a	0.165297	0.233828	0.09695	0.0285
N3a	0.327226	0.415477	0.302297	0.0505
C1a	0.094(5)	0.667(6)	0.258(4)	0.028
C2a	0.065(5)	0.785(6)	0.306(4)	0.0331
C3a	0.013(5)	0.799(6)	0.393(4)	0.031
C4a	-0.003(5)	0.695(6)	0.431(4)	0.0246
C5a	0.028(5)	0.578(6)	0.378(4)	0.0233
C6	0.144(8)	0.645(9)	0.160(4)	0.0264
C7	-0.026(10)	0.756(7)	0.534(4)	0.0264
C8a	0.197605	0.225305	0.007392	0.0372
C9a	0.2248	0.112572	-0.051338	0.0494
C10a	0.221651	0.005724	-0.016115	0.0534
C11a	0.193489	0.015117	0.077827	0.0451
C12a	0.164291	0.130282	0.131194	0.0315
C13	0.182(10)	0.172(8)	0.247(2)	0.0264
C14a	0.30261	0.292371	0.313931	0.0505
C15a	0.432171	0.249022	0.363632	0.0505
C16a	0.586323	0.328674	0.401688	0.0505
C17a	0.610938	0.45178	0.390054	0.0505
C18a	0.481378	0.495129	0.340354	0.0505
C19a	-0.291(9)	0.460(8)	0.062(6)	0.0477
C20a	-0.285(9)	0.370(8)	0.127(6)	0.0498
C22a	0.524889	0.836865	0.434883	0.0519
C23a	0.499995	0.877956	0.346992	0.061

Table S16.- Geometric parameters (Å, º) for compound **3e**.

Ni1-O1	2.04(15)	N3A-C18A	1.3751
Ni1-O5	2.14(16)	C1A-C2A	1.35(9)
Ni1-O7A	2.08(10)	C1A-C6	1.50(8)
Ni1-N1A	2.07(8)	C2A-C3A	1.37(7)
Ni1-N2A	2.0709	C3A-C4A	1.41(9)
Ni1-N3A	2.0826	C4A-C5A	1.37(9)
O1 -C6	1.25(16)	C4A-C7	1.48(8)
O2 -C6	1.26(18)	C8A-C9A	1.3473
O3 -C7	1.28(14)	C9A-10A	1.4127
O4 -C7	1.24(12)	C10A-C11A	1.3827
O5 -C13	1.41(18)	C11A-C12A	1.3487
O6 -C13	1.41(16)	C12A-C13	1.5475
O7A-C20A	1.41(11)	C13-C14A	1.4834
N1A-C1A	1.37(9)	C14A-C15A	1.4083

N1A-C5A	1.33(7)	C15A-C16A	1.3751
N2A-C8A	1.3367	C16A-C17A	1.4081
N2A-C12A	1.3706	C17A-C18A	1.4083
N3A-C14A	1.4081	C19A-C20A	1.55(12)
Ni1-O1	2.04(15)	N3A-C18A	1.3751

O1-Ni1-O5	173(7)	C3A-C4A-C5A	119(5)
O1-Ni1-O7A	114(5)	C3A-C4A-C7	104(5)
O1-Ni1-N1A	81(5)	C5A-C4A-C7	136(6)
O1-Ni1-N2A	106.91	N1A-C5A-C4A	120(6)
O1-Ni1-N3A	103.17	O1-C6-O2	127(10)
O5-Ni1-O7A	73(6)	O1-C6-C1A	114(9)
O5-Ni1-N1A	102(5)	O2-C6-C1A	119(9)
O5-Ni1-N2A	70.36	O3-C7-O4	127(8)
O5-Ni1-N3A	70.32	O3-C7-C4A	119(8)
O7A-Ni1-N1A	85(3)	O4-C7-C4A	114(7)
O7A-Ni1-N2A	91.59	N2A-C8A-C9A	119.75
O7A-Ni1-N3A	140.07	C8A-C9A-C10A	119.20
N1A-Ni1-N2A	171.78	C9A-C10A-C11A	121.36
N1A-Ni1-N3A	87.93	C10A-C11A-C12A	115.84
N2A-Ni1-N3A	90.07	N2A-C12A-C11A	123.06
Ni1-O1-C6	112(10)	N2A-C12A-C13	112.23
Ni1-O5-C13	115(11)	C11A-C12A-C13	122.04
Ni1-O7A-C20A	147(7)	O5-C13-O6	114(10)
Ni1-N1A-C1A	108(4)	O5-C13-C12A	95.78
Ni1-N1A-C5A	132(5)	O5-C13-C14A	83.88
C1A-N1A-C5A	120(6)	O6-C13-C12A	110.70
Ni1-N2A-C8A	120.28	O6-C13-C14A	125.31
Ni1-N2A-C12A	118.93	C12A-C13-C14A	118.74
C8A-N2A-C12A	120.74	N3A-C14A-C13	128.21
Ni1-N3A-C14A	105.40	N3A-C14A-C15A	121.52
Ni1-N3A-C18A	132.44	C13-C14A-C15A	105.15
C14A-N3A-C18A	119.20	C14A-C15A-C16A	119.28
N1A-C1A-C2A	123(5)	C15A-C16A-C17A	119.20
N1A-C1A-C6	118(6)	C16A-C17A-C18A	121.52
C2A-C1A-C6	119(6)	N3A-C18A-C17A	119.28
C1A-C2A-C3A	117(6)	O7A-C20A-C19A	110(7)
C2A-C3A-C4A	120(6)		

Table S17.- Fractional atomic coordinates and isotropic (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **3p**.

Atom	x	y	z	U(eq) [Ang^2]
Ni(1)	1034(1)	3954(1)	1889(1)	24(1)
O(1)	1805(4)	5103(3)	1110(2)	33(1)
O(2)	1794(5)	7070(3)	938(2)	39(1)
O(3)	-145(4)	6728(3)	5608(2)	31(1)
O(4)	-971(5)	8479(3)	5336(3)	40(1)
O(5)	361(4)	2516(3)	2555(2)	27(1)
O(6)	1573(5)	833(3)	2899(3)	46(1)
O(7)	-1373(4)	3616(4)	1040(2)	36(1)
O(8)	6650(30)	10160(20)	4134(18)	151(9)
O(8A)	6757(19)	10207(15)	2996(12)	111(5)
N(1)	760(5)	5694(3)	2778(3)	26(1)
N(2)	1476(5)	2327(3)	960(3)	30(1)
N(3)	3234(3)	4032(3)	2884(2)	52(1)
C(1)	1016(6)	6631(4)	2343(3)	30(1)

C(2)	800(7)	7866(4)	2748(3)	35(1)
C(3)	313(6)	8153(4)	3638(3)	33(1)
C(4)	104(5)	7208(4)	4115(3)	26(1)
C(5)	339(5)	5985(4)	3656(3)	25(1)
C(6)	1573(6)	6238(4)	1376(3)	32(1)
C(7)	-377(5)	7495(4)	5101(3)	26(1)
C(8)	1525(7)	2067(5)	-9(4)	38(1)
C(9)	1825(8)	912(5)	-532(4)	51(2)
C(10)	2121(9)	7(5)	-33(5)	55(2)
C(11)	2123(8)	285(5)	982(4)	47(1)
C(12)	1779(6)	1449(4)	1440(4)	33(1)
C(13)	1729(6)	1890(4)	2551(3)	33(1)
C(14)	3231(3)	2876(3)	3113(3)	52(1)
C(15)	4596(4)	2717(3)	3769(3)	52(1)
C(16)	5963(3)	3714(4)	4197(3)	52(1)
C(17)	5965(3)	4870(3)	3968(3)	52(1)
C(18)	4601(4)	5029(3)	3311(3)	52(1)
C(19)	-3216(12)	5121(10)	1165(8)	56(2)
C(19A)	-3670(40)	4710(30)	1070(30)	56(2)
C(20)	-2777(7)	3892(6)	1396(5)	51(1)
C(21)	-4102(10)	2788(8)	1024(7)	56(2)
C(21A)	-3370(30)	2920(30)	1850(20)	56(2)
C(22)	4507(17)	8250(10)	3908(9)	55(3)
C(22A)	6745(19)	10038(14)	4653(11)	48(3)
C(23)	5230(20)	9026(16)	3372(14)	65(4)
C(23A)	5860(30)	9620(20)	3633(15)	58(4)
C(24)	5721(18)	8231(14)	2521(12)	73(4)
C(24A)	5570(20)	8181(18)	3342(14)	76(5)

Table S18.- Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **3p**.

Atom	**U(1,1)**	**U(2,2)**	**U(3,3)**	**U(2,3)**	**U(1,3)**	**U(1,2)**
Ni1	34(1)	21(1)	21(1)	7(1)	13(1)	8(1)
O1	53(2)	24(2)	30(2)	12(1)	23(2)	11(1)
O2	70(2)	25(2)	26(2)	10(1)	22(2)	8(2)
O3	50(2)	24(1)	23(2)	9(1)	15(1)	11(1)
O4	66(2)	34(2)	36(2)	16(2)	28(2)	23(2)
O5	38(2)	23(1)	24(2)	8(1)	14(1)	7(1)
O6	81(3)	30(2)	39(2)	15(2)	30(2)	21(2)
O7	34(2)	57(2)	22(2)	13(2)	12(1)	16(2)
O8	129(13)	127(13)	156(17)	10(12)	-11(12)	29(10)
O8A	110(10)	127(11)	113(10)	42(8)	55(8)	32(8)
N1	38(2)	23(2)	23(2)	10(1)	11(2)	9(2)
N2	41(2)	25(2)	28(2)	6(2)	18(2)	8(2)
N3	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)
C1	45(3)	25(2)	25(2)	10(2)	13(2)	11(2)
C2	61(3)	26(2)	28(2)	15(2)	20(2)	12(2)
C3	54(3)	21(2)	26(2)	7(2)	15(2)	13(2)
C4	34(2)	23(2)	23(2)	9(2)	9(2)	7(2)
C5	35(2)	23(2)	18(2)	7(2)	9(2)	6(2)
C6	46(3)	24(2)	27(2)	10(2)	12(2)	7(2)
C7	35(2)	19(2)	24(2)	6(2)	10(2)	5(2)
C8	56(3)	34(3)	30(2)	8(2)	23(2)	10(2)
C9	82(4)	43(3)	38(3)	9(2)	36(3)	18(3)
C10	89(5)	33(3)	56(3)	7(2)	48(3)	20(3)
C11	73(4)	32(3)	51(3)	15(2)	39(3)	22(3)
C12	47(3)	24(2)	34(2)	9(2)	23(2)	9(2)
C13	50(3)	25(2)	31(2)	11(2)	21(2)	18(2)
C14	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)
C15	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)

C16	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)
C17	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)
C18	39(1)	59(1)	51(1)	4(1)	9(1)	14(1)
C19	45(3)	65(4)	55(3)	5(3)	19(3)	14(3)
C19A	45(3)	65(4)	55(3)	5(3)	19(3)	14(3)
C20	45(3)	76(4)	51(3)	27(3)	28(3)	27(3)
C21	45(3)	65(4)	55(3)	5(3)	19(3)	14(3)
C21A	45(3)	65(4)	55(3)	5(3)	19(3)	14(3)
C22	85(8)	33(5)	48(6)	12(5)	23(6)	7(5)
C22A	47(7)	41(6)	53(8)	6(6)	16(6)	9(5)
C23	82(10)	41(8)	75(10)	28(7)	18(8)	10(7)
C23A	67(10)	54(10)	70(10)	25(8)	34(9)	35(8)
C24	66(8)	72(8)	76(9)	11(7)	22(7)	12(7)

Table S19.- Geometric parameters (Å, º) for compound **3p**.

Ni1-N1	2.070(3)	C11-C12	1.376(7)
Ni1-N2	2.058(4)	C12-N2	1.339(6)
Ni1-N3	2.071(2)	C12-C13	1.534(6)
Ni1-O1	2.012(3)	C13-O6	1.376(6)
Ni1-O5	2.116(3)	C13-O5	1.435(5)
Ni1-O7	2.077(3)	C13-C14	1.479(6)
O8-C23	1.59(3)	C14-C15	1.3900
C1-N1	1.348(5)	C14-N3	1.3900
C1-C2	1.382(6)	C15-C16	1.3900
C1-C6	1.521(6)	C16-C17	1.3900
C2-C3	1.384(6)	C17-C18	1.3900
C3-C4	1.390(6)	C18-N3	1.3900
C4-C5	1.393(6)	C20-C19A	1.36(4)
C4-C7	1.507(6)	C20-O7	1.436(6)
C5-N1	1.339(5)	C20-C21	1.437(10)
C6-O2	1.245(5)	C20-C21A	1.47(3)
C6-O1	1.261(5)	C20-C19	1.546(12)
C7-O3	1.252(5)	C22-C23	1.440(19)
C7-O4	1.253(5)	C23-C24	1.47(2)
C8-N2	1.339(6)	O8A-C23A	1.51(2)
C8-C9	1.380(7)	C24A-C23A	1.50(2)
C9-C10	1.382(8)	C22A-C23A	1.40(3)
C10-C11	1.391(8)		

O1-C6-C1	116.3(4)	N2-Ni1-N1	174.43(14)
O1-Ni1-N1	81.22(13)	N2-Ni1-N3	86.56(15)
O1-Ni1-N2	93.72(13)	N2-Ni1-O5	77.16(13)
O1-Ni1-N3	100.20(15)	N2-Ni1-O7	92.41(15)
O1-Ni1-O5	170.81(12)	N3-C14-C13	113.3(3)
O1-Ni1-O7	91.81(14)	N3-C18-C17	120.0
O2-C6-C1	117.4(4)	N3-Ni1-O5	78.38(13)
O2-C6-O1	126.3(4)	N3-Ni1-O7	167.99(14)
O3-C7-C4	116.9(4)	C12-N2-C8	118.5(4)
O3-C7-O4	126.1(4)	C12-N2-Ni1	112.3(3)
O4-C7-C4	117.0(4)	C13-O5-Ni1	100.2(2)
O5-C13-C12	105.3(4)	C14-N3-Ni1	110.35(18)
O5-C13-C14	107.7(3)	C15-C14-N3	120.0
O6-C13-C12	108.9(4)	C18-N3-C14	120.0
O6-C13-C14	113.9(4)	C18-N3-Ni1	129.65(18)
O6-C13-O5	113.2(4)	C19A-C20-O7	121.4(15)
O7-C20-C19	109.3(5)	C1-N1-Ni1	110.8(3)

O7-C20-C21	111.6(5)	C20-O7-Ni1	127.8(3)
O7-C20-C21A	111.3(11)	C21A-C20-C19	139.3(11)
O7-Ni1-O5	89.71(13)	C21-C20-C19	114.8(6)
N1-C1-C2	122.5(4)	C22A-C23A-O8A	111.3(18)
N1-C1-C6	115.3(4)	C22-C23-O8	110.8(16)
N1-C5-C4	122.3(4)	C24A-C23A-O8A	114.2(14)
N1-Ni1-N3	92.04(14)	C24-C23-O8	114.0(17)
N1-Ni1-O5	107.85(13)	C5-N1-C1	118.6(4)
N1-Ni1-O7	90.07(14)	C5-N1-Ni1	130.5(3)
N2-C12-C11	123.2(4)	C6-O1-Ni1	115.3(3)
N2-C12-C13	112.9(4)	C8-N2-Ni1	129.2(3)
N2-C8-C9	122.1(5)		