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Template synthesis of Ni(II) complexes of unsymmetrical Schiff base ligands derived from 1,3-diamino-2-propanol: structural diversity and magnetic properties

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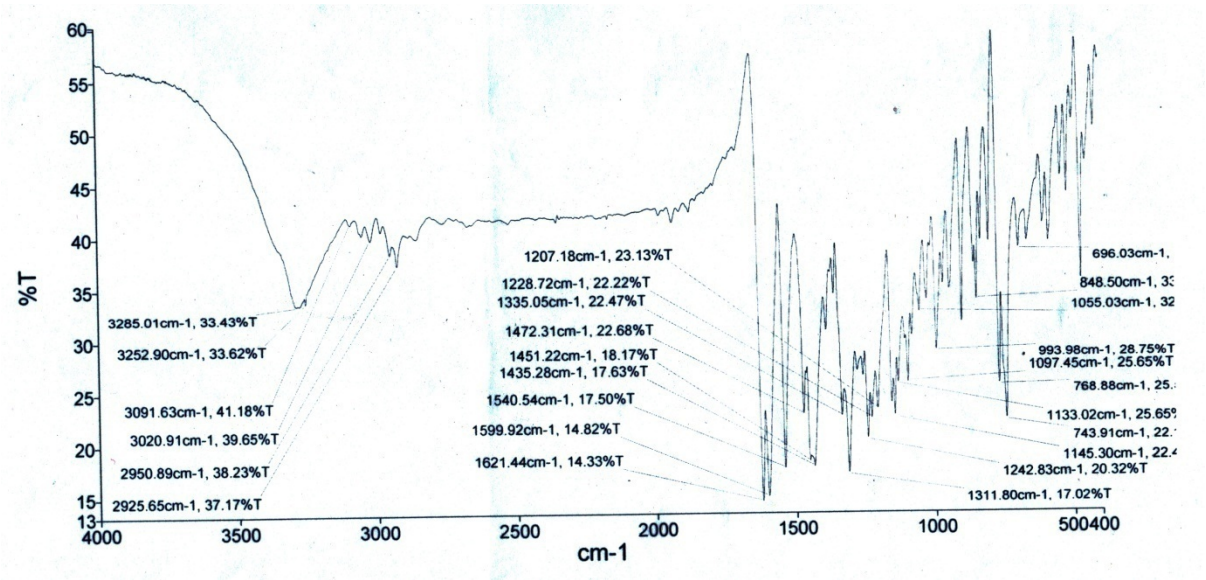

Fig. S1 IR spectrum of complex **1**

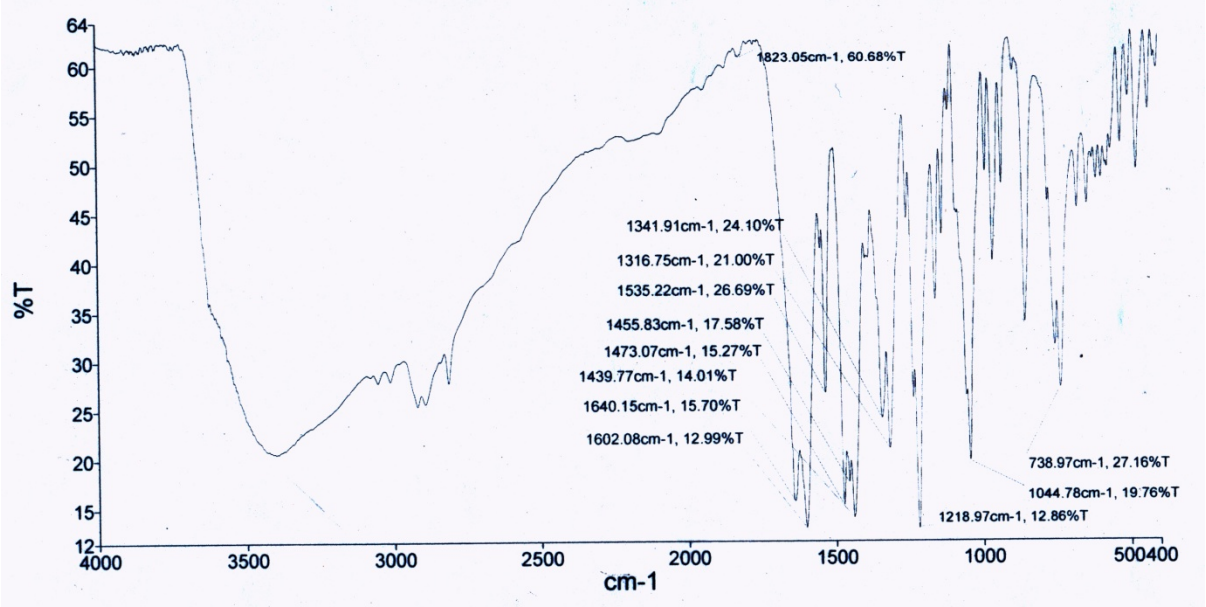

Fig. S2 IR spectrum of complex **2**

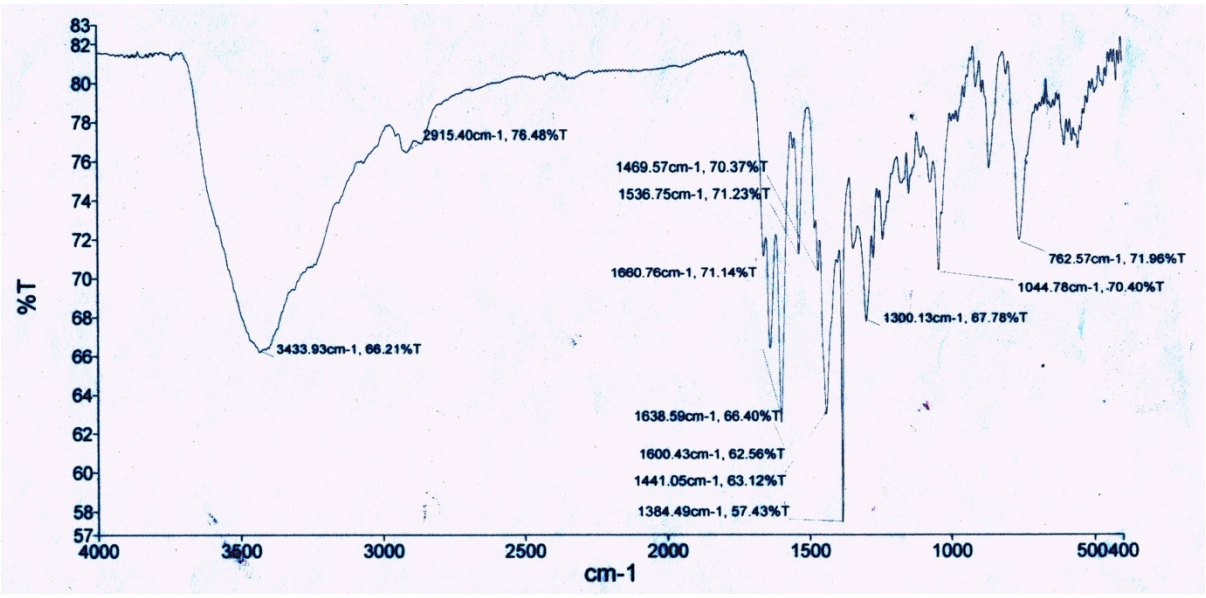

Fig. S3 IR spectrum of complex **3**

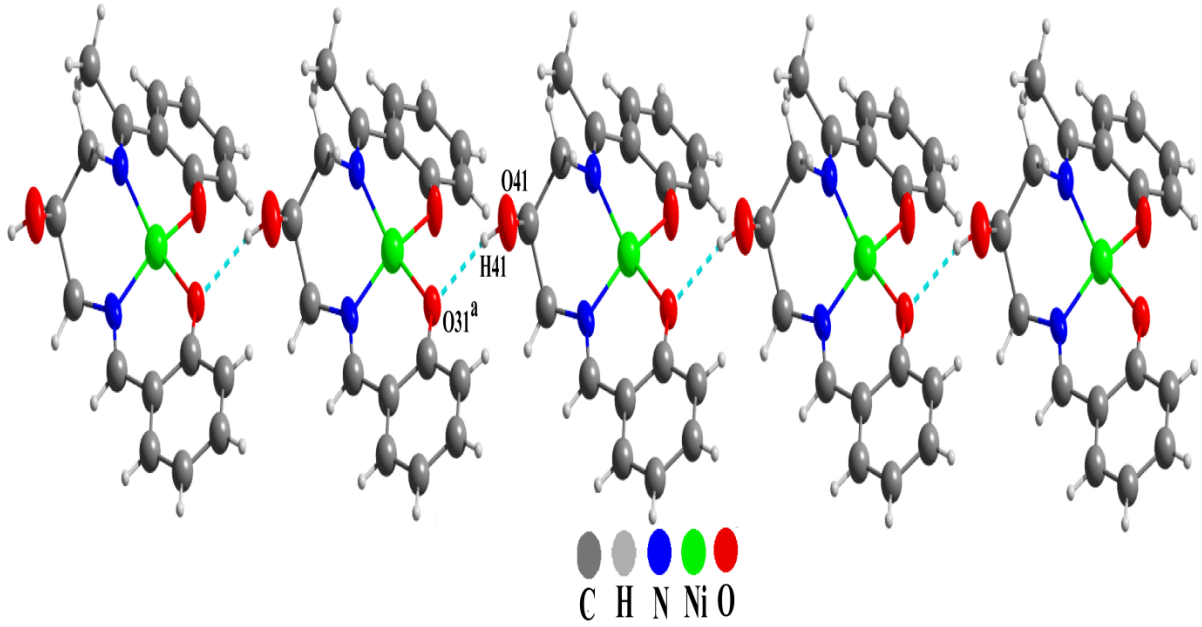

Fig. S4 H-bonded structure of complex **1**. H-bonds are shown by dotted lines.

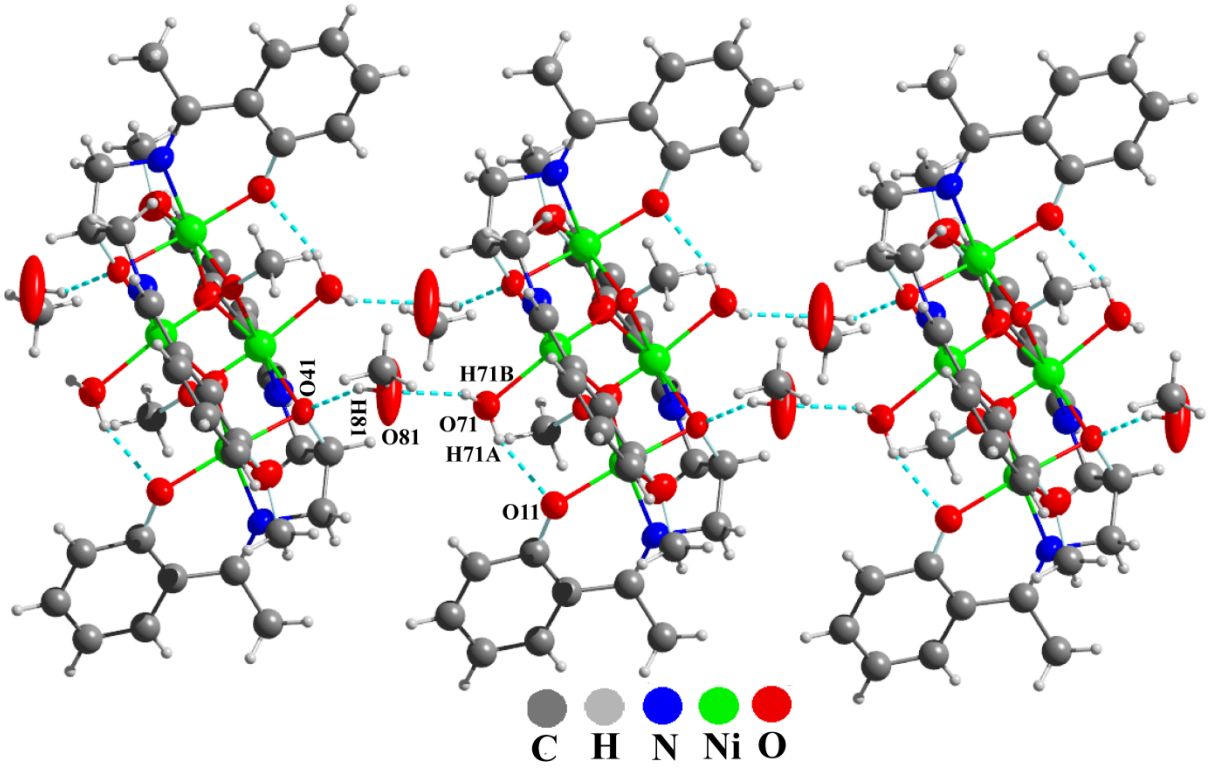

Fig. S5 H-bonded structure of complex **2**. H-bonds are shown by dotted lines.

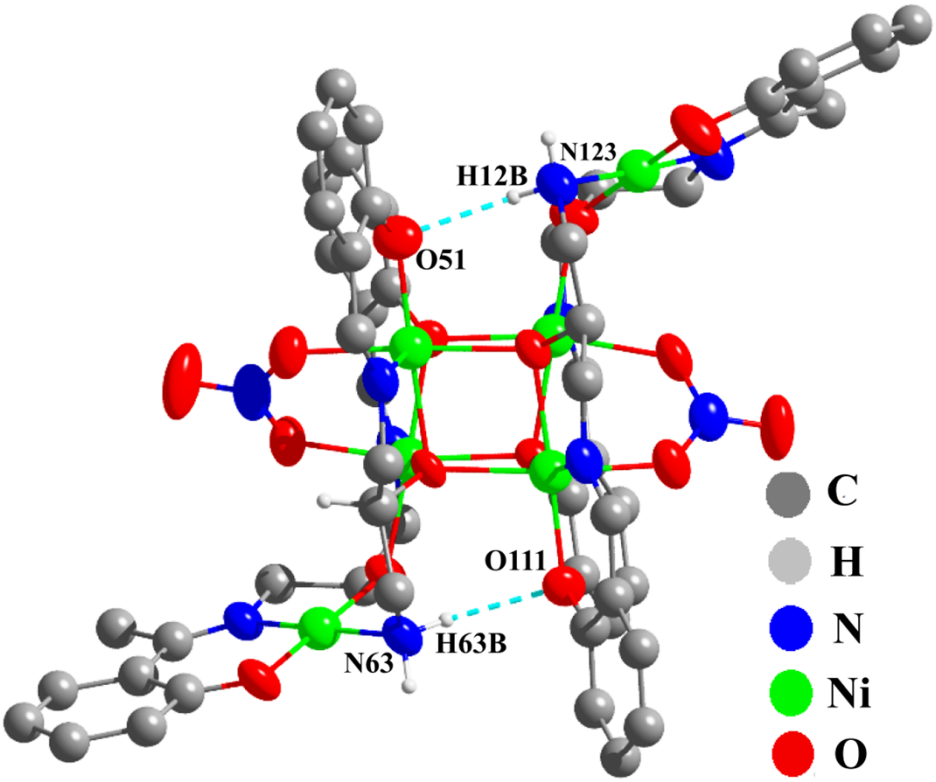

Fig. S6 H-bonded structure of complex **3**. H-bonds are shown by dotted lines.

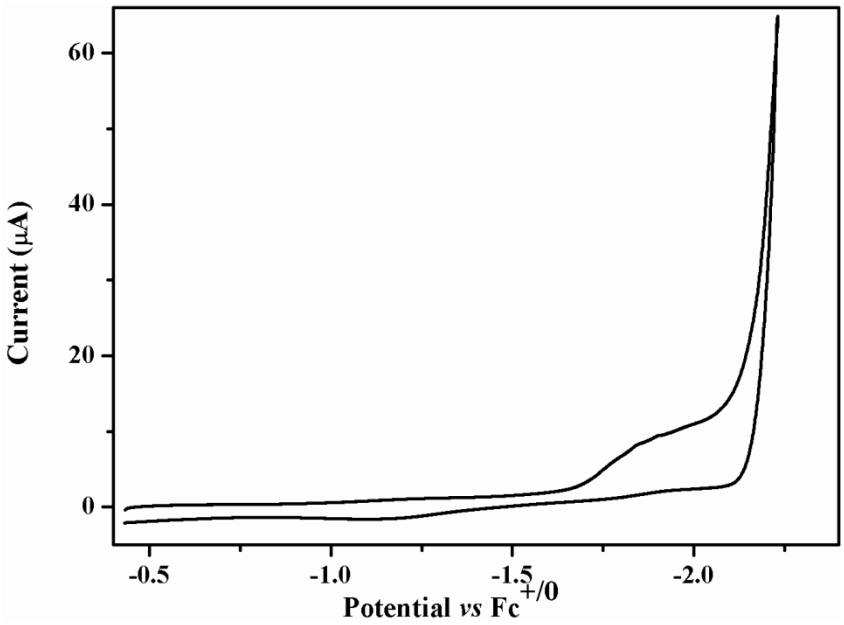

Fig. S7 Cyclic voltammograms of zinc complex was recorded in acetonitrile (0.1 M TBAP) at a scan rate of 100 mVs^{-1}.

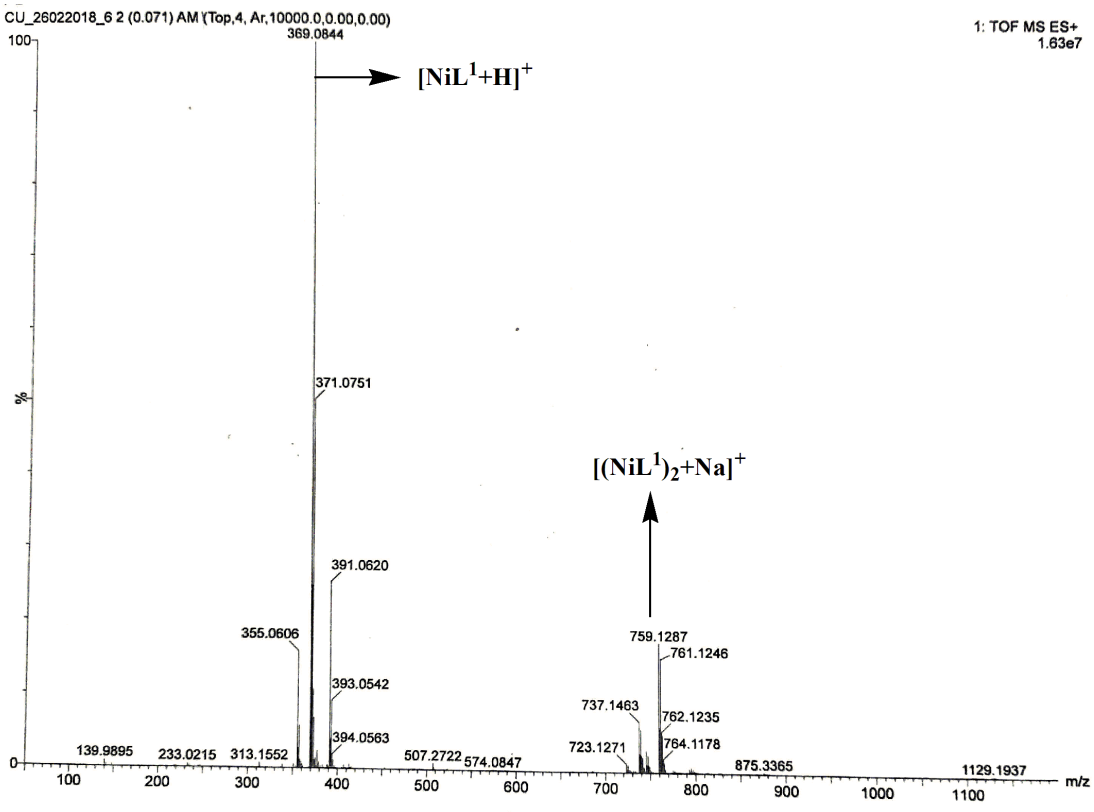

Fig. S8 ESI-MS spectrum of complex **1**.

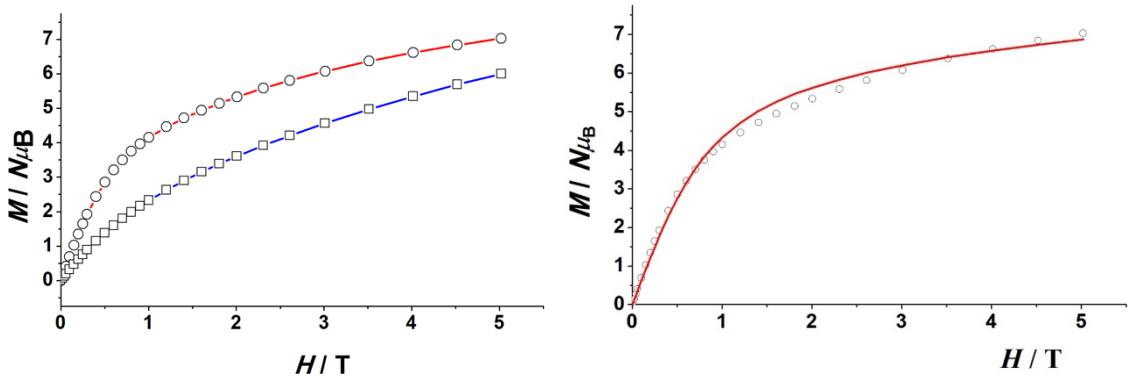

Fig. S9 Magnetization vs. field for complexes **2** (black circles) and **3** (black squares) showing low magnetization curves (left) and Fit of the magnetization for complex 2 (right).

Table S1 Selected bond lengths (Å) and bond angles (°) of Complex **1**

Bond lengths (Å)		**Bond angles (°)**	
Ni(1) – O(11)	1.831(2)	O(11) – Ni(1) – O(31)	85.27(7)
Ni(1) – O(31)	1.856(2)	O(11) – Ni(1) – N(19)	92.47(8)
Ni(1) – N(19)	1.880(2)	O(11) – Ni(1) – N(23)	163.17(8)
Ni(1) – N(23)	1.873(2)	O(31) – Ni(1) – N(19)	163.17(8)
		O(31) – Ni(1) – N(23)	94.90(7)
		N(19) – Ni(1) – N(23)	91.98(8)

Table S2 Selected bond lengths (Å) and bond angles (°) of Complex **2**

Bond lengths (Å)			
Ni(1) – O(11)	1.986(2)	Ni(2) – O(31)	2.020(2)
Ni(1) – O(41)	2.060(2)	Ni(2) – O(41)	2.065(2)
Ni(1) – O(51)	2.044(2)	Ni(2) – O(51)	2.059(3)
Ni(1) – N(19)	2.008(3)	Ni(2) – O(71)	2.089(2)
Ni(1) – O(31^{a})	1.995(2)	Ni(2) – N(23)	1.989(3)
Ni(1) – O(61^{a})	2.403(3)	Ni(2) – O(51^{a})	2.062(2)
Bond angles (°)			
O(11) – Ni(1) – O(41)	172.80(10)	O(31) – Ni(2) – O(41)	167.78(8)
O(11) – Ni(1) – O(51)	96.12(8)	O(31) – Ni(2) – O(51)	89.01(8)
O(11) – Ni(1) – N(19)	90.51(10)	O(31) – Ni(2) – O(71)	91.23 (9)
O(11) – Ni(1) – O(31^{a})	90.90(9)	O(31) – Ni(2) – N(23)	88.89(10)
O(11) – Ni(1) – O(61^{a})	83.72(10)	O(31) – Ni(2) – O(51^{a})	79.56(8)
O(41) – Ni(1) – O(51)	82.04(8)	O(41) – Ni(2) – O(51)	81.58(8)
O(41) – Ni(1) – N(19)	83.94(10)	O(41) – Ni(2) – O(71)	99.39(8)
O(31^{a}) – Ni(1) – O(41)	95.64(8)	O(41) – Ni(2) – N(23)	84.46(10)
O(41) – Ni(1) – O(61^{a})	101.23(9)	O(41) – Ni(2) – O(51^{a})	107.19(8)
O(51) – Ni(1) – N(19)	114.05(10)	O(51) – Ni(2) – O(71)	170.08(9)
O(31^{a}) – Ni(1) – O(51)	80.58(8)	O(51) – Ni(2) – N(23)	96.40(10)
O(51) – Ni(1) – O(61^{a})	151.54(8)	O(51) – Ni(2) – O(51^{a})	85.05(8)
O(31^{a}) – Ni(1) – N(19)	165.05(10)	O(71) – Ni(2) – N(23)	93.51(11)
O(61^{a}) – Ni(1) – N(19)	94.40(10)	O(51^{a}) – Ni(2) – O(71)	85.24(9)
O(31^{a}) – Ni(1) – N(61^{a})	70.98(9)	O(51^{a}) – Ni(2) – N(23)	168.35(10)

Table S3 Selected bond lengths (Å) of Complex **3**

Bond lengths (Å)			
Ni(1) – O(11)	1.822(3)	Ni(4) – O(71)	1.812(5)
Ni(1) – O(41)	1.843(3)	Ni(4) – O(101)	1.848(3)
Ni(1) – N(19)	1.846(5)	Ni(4) – N(79)	1.838(5)
Ni(1) – N(63)	1.906(5)	Ni(4) – N(123)	1.900(5)
Ni(2) – O(31)	2.087(3)	Ni(5) – O(31)	2.140(3)
Ni(2) – O(41)	2.042(3)	Ni(5) – O(91)	2.083(3)
Ni(2) – O(61)	2.060(3)	Ni(5) – O(101)	2.058(3)
Ni(2) – O(91)	2.135(3)	Ni(5) – O(121)	2.059(3)
Ni(2) – O(131)	2.094(4)	Ni(5) – O(141)	2.110(4)
Ni(2) – N(23)	1.993(5)	Ni(5) – N(83)	1.996(5)
Ni(3) – O(31)	2.121(3)	Ni(6) – O(61)	2.095(3)
Ni(3) – O(51)	1.943(4)	Ni(6) – O(91)	2.136(3)
Ni(3) – O(61)	2.096(3)	Ni(6) – O(111)	1.968(4)
Ni(3) – O(121)	2.093(3)	Ni(6) – O(121)	2.121(3)
Ni(3) – O(132)	2.144(4)	Ni(6) – O(142)	2.129(4)
Ni(3) – N(59)	1.999(5)	Ni(6) – N(119)	2.001(5)

Table S4 Selected bond angles (°) of Complex **3**

Bond angles (°)			
O(11) – Ni(1) – O(41)	175.35(15)	O(71) – Ni(4) – O(101)	175.19(19)
O(11) – Ni(1) – N(19)	96.12(18)	O(71) – Ni(4) – N(79)	95.8(2)
O(11) – Ni(1) – N(63)	86.69(18)	O(71) – Ni(4) – N(123)	87.0(2)
O(41) – Ni(1) – N(19)	88.22(18)	O(101) – Ni(4) – N(79)	88.75(19)
O(41) – Ni(1) – N(63)	89.03(18)	O(101) – Ni(4) – N(123)	88.57(18)
N(19) – Ni(1) – N(63)	176.6(2)	N(79) – Ni(4) – N(123)	175.1(2)
O(31) – Ni(2) – O(41)	172.63(12)	O(31) – Ni(5) – O(91)	79.15(13)
O(31) – Ni(2) – O(61)	87.93(12)	O(31) – Ni(5) – O(101)	101.53(14)
O(31) – Ni(2) – O(91)	79.20(13)	O(31) – Ni(5) – O(121)	81.23(12)
O(31) – Ni(2) – O(131)	90.39(15)	O(31) – Ni(5) – O(141)	168.18(14)
O(31) – Ni(2) – N(23)	90.51(16)	O(31) – Ni(5) – N(83)	95.09(17)
O(41) – Ni(2) – O(61)	99.43(13)	O(91) – Ni(5) – O(101)	172.76(12)
O(41) – Ni(2) – O(91)	102.15(13)	O(91) – Ni(5) – O(121)	88.76(12)
O(41) – Ni(2) – O(131)	88.74(15)	O(91) – Ni(5) – O(141)	90.03(14)
O(41) – Ni(2) – N(23)	82.16(17)	O(91) – Ni(5) – N(83)	90.69(15)
O(61) – Ni(2) – O(91)	81.25(12)	O(101) – Ni(5) – O(121)	98.48(13)
O(61) – Ni(2) – O(131)	94.06(16)	O(101) – Ni(5) – O(141)	89.80(15)
O(61) – Ni(2) – N(23)	176.46(17)	O(101) – Ni(5) – N(83)	82.07(16)
O(91) – Ni(2) – O(131)	168.68(15)	O(121) – Ni(5) – O(141)	93.91(13)
O(91) – Ni(2) – N(23)	95.33(17)	O(121) – Ni(5) – N(83)	176.32(18)
O(131) – Ni(2) – N(23)	89.1(2)	O(141) – Ni(5) – N(83)	89.74(17)
O(31) – Ni(3) – O(51)	99.47(13)	O(61) – Ni(6) – O(91)	80.42(12)

O(31) – Ni(3) – O(61)	86.09(12)	O(61) – Ni(6) – O(111)	98.18(14)
O(31) – Ni(3) – O(121)	80.93(12)	O(61) – Ni(6) – O(121)	80.33(13)
O(31) – Ni(3) – O(132)	85.85(15)	O(61) – Ni(6) – O(142)	164.95(12)
O(31) – Ni(3) – N(59)	165.97(17)	O(61) – Ni(6) – N(119)	107.47(17)
O(51) – Ni(3) – O(61)	173.99(13)	O(91) – Ni(6) – O(111)	100.26(13)
O(51) – Ni(3) – O(121)	97.59(14)	O(91) – Ni(6) – O(121)	85.77(12)
O(51) – Ni(3) – O(132)	88.34(16)	O(91) – Ni(6) – O(142)	84.87(12)
O(51) – Ni(3) – N(59)	91.84(17)	O(91) – Ni(6) – N(119))	164.78(16)
O(61) – Ni(3) – O(121)	80.95(13)	O(111) – Ni(6) – O(121)	173.50(12)
O(61) – Ni(3) – O(132)	94.37(15)	O(111) – Ni(6) – O(142)	87.51(15)
O(61) – Ni(3) – N(59)	83.00(16)	O(111) – Ni(6) – N(119)	91.61(16)
O(121) – Ni(3) – O(132)	166.22(15)	O(121) – Ni(6) – O(142)	95.50(14)
O(121) – Ni(3) – N(59)	105.92(17)	O(121) – Ni(6) – N(119)	82.87(16)
O(132) – Ni(3) – N(59)	86.22(19)	O(142) – Ni(6) – N(119)	86.16(17)

Table S5 Geometrical features of hydrogen bonding interactions (distances (Å) and angles (°)) of Complexes **1**, **2** and **3**

Complex	D−H···A	D−H (Å)	H···A (Å)	D···A (Å)	∠D−H···A (°)
1	O(41) – H(41) ··· O(31)	0.82	2.03	2.841(2)	173
2	O(71) – H(71A) ··· O(11)	0.88	1.97	2.786(3)	154
	O(71) – H(71B) ··· O(81)	0.88	1.89	2.638(4)	143
	O(81) – H(81) ··· O(41)	0.82	1.84	2.633(4)	161
3	N(123) – H(12B) ··· O(51)	0.89	2.14	2.874(6)	139
	N(63) – H(63B) ··· O(111)	0.89	2.17	2.899(6)	138