Electronic Supplementary Material (ESI) for CrystEngComm.
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Effect of N-Salicylidene hydrazide protonation on the solid state structural diversity of its Cu(II), Ni(II) and Zn(II) complexes.

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Suplementary Information

Table S1. Crystal and structure refinement data.

Compound	**H_2L**	**Zn-1a**	**Cu-3a**	**Cu-3b**	**Ni-3a**	**NiL***
Empirical formula	$C_{13}H_{18}N_2O_3$	$C_{28}H_{41}N_5O_{10}Zn$	$C_{26}H_{34}N_6O_{12}Cu_2$	$C_{26}H_{32}N_4O_6F_6SiCu_2$	$C_{30}H_{50}N_6O_{16}Ni_2$	C_{32} $H_{30}N_4O_9Ni$
Formula weigth	250.29	673.03	749.67	765.72	868.18	673.31
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P2₁/c*	*P-1*	*P2₁/c*	*C2/m*	*P-1*	*C2/c*
CCDC ref.	1858827	1858828	1858829	1858830	1858831	1858832
a (Å)	5.3989(3)	13.6157(14)	11.8828(4)	15.2574(3)	9.4517(14)	22.063(9)
b (Å)	10.1581(5)	14.5331(16)	7.2916(2)	7.15810(10)	10.1415(14)	5.803(2))
c (Å)	23.3868(12)	18.1322(19)	17.5807(6)	13.6618(3)	10.5338(15)	24.656(10)
α (º)	90	109.291(3)	90	90	107.386(7)	90
β (º)	90.5082(17)	110.987(3)	92.6591(6)	102.2698(6)	91.631(8)	105.727(7)
γ (º)	90	95.422(3)	90	90	92.042(8)	90
V (Å^3)	1282.54(12)	3068.3(6)	1521.63(8)	1457.98(5)	962.2(2)	3039(2)
Z	4	4	2	2	2	4
λ(Å)	1.54178	0.71073	1.54178	1.54178	1.54178	0.71073
T (K)	296(2)	100(2)	293(2)	296(2)	293(2)	293(2)
ρ_{calcd} (g cm^{-3})	1.296	1.457	1.636	1.744	1.498	0.701
μ (mm^{-1})	0.761	0.864	2.364	2.987	1.887	1.472
F(000)	536	1416	772	780	456	1400
Indep. ref.(R_{int})	2337 (0.0267)	12636 (0.0532)	2766 (0.0231)	1389 (0.0348)	3362 (0.0993)	3701 (0.0718)
final *R* indices	R_1= 0.0798	R_1= 0.0901	R_1= 0.0297	R_1= 0.0334	R_1= 0.0887	R_1= 0.0703
[*I*> 2σ(*I*)]	wR_2= 0.3049	wR_2= 0.2300	wR_2= 0.0867	wR_2= 0.0948	wR_2= 0.2411	wR_2= 0.1724

Table S2. Selected bond lengths (Å) and bond angles (°)

- *Compound H_2L*

DISTANCES		ANGLES	
O(1)-C(8)	1.241(3)	C(8)-N(2)-N(1)	121.29(18)
N(2)-C(8)	1.341(3)	C(1)-N(1)-N(2)	116.51(17)
N(2)-N(1)	1.373(3)	O(1)-C(8)-N(2)	118.74(18)
N(1)-C(1)	1.282(3)	O(1)-C(8)-C(9)	122.15(18)
C(8)-C(9)	1.502(3)	N(2)-C(8)-C(9)	119.11(18)
C(2)-C(3)	1.402(3)	C(3)-C(2)-C(7)	118.8(2)
C(2)-C(7)	1.403(3)	C(3)-C(2)-C(1)	122.10(19)
C(2)-C(1)	1.456(3)	C(7)-C(2)-C(1)	119.09(19)
O(2)-C(13)	1.416(3)	N(1)-C(1)-C(2)	120.67(18)
C(7)-C(6)	1.378(3)	C(6)-C(7)-C(2)	120.8(2)
C(3)-O(3)	1.343(4)	O(3)-C(3)-C(4)	118.4(2)
C(3)-C(4)	1.389(3)	O(3)-C(3)-C(2)	122.0(2)
C(9)-C(10)	1.516(3)	C(4)-C(3)-C(2)	119.6(2)
C(6)-C(5)	1.385(4)	C(8)-C(9)-C(10)	114.26(17)
C(5)-C(4)	1.379(4)	C(7)-C(6)-C(5)	119.9(2)
C(10)-C(11)	1.527(3)	C(4)-C(5)-C(6)	120.1(2)
C(13)-C(12)	1.508(3)	C(9)-C(10)-C(11)	110.04(18)
C(12)-C(11)	1.521(3)	C(5)-C(4)-C(3)	120.8(2)
		O(2)-C(13)-C(12)	115.0(2)
		C(13)-C(12)-C(11)	112.73(19)
		C(12)-C(11)-C(10)	113.02(19)

- *Compound Zn-1a*

DISTANCES		ANGLES	
O(51)-N(21)	1.224(8)	O(51)-N(21)-O(53)	120.4(7)
N(21)-O(53)	1.234(8)	O(51)-N(21)-O(52)	120.2(7)
N(21)-O(52)	1.257(9)	O(53)-N(21)-O(52)	119.3(6)
O(55)-N(20)	1.204(8)	O(55)-N(20)-O(54)	121.8(6)
N(20)-O(54)	1.257(7)	O(55)-N(20)-O(56)	120.9(6)
N(20)-O(56)	1.275(7)	O(54)-N(20)-O(56)	117.2(6)
C(64)-C(63)	1.475(12)	O(15)-C(63)-C(64)	112.6(7)
C(63)-O(15)	1.431(8)	O(40)-C(61)-C(60)	115.2(7)
C(60)-C(61)	1.467(12)	O(8)-Zn(1)-O(7)	88.88(16)
C(61)-O(40)	1.415(9)	O(8)-Zn(1)-N(5)	83.33(17)
Zn(1)-O(8)	2.076(4)	O(7)-Zn(1)-N(5)	104.70(17)
Zn(1)-O(7)	2.089(4)	O(8)-Zn(1)-N(7)	103.29(16)
Zn(1)-N(5)	2.106(5)	O(7)-Zn(1)-N(7)	82.23(16)
Zn(1)-N(7)	2.116(4)	N(5)-Zn(1)-N(7)	170.67(18)
Zn(1)-O(4)	2.117(4)	O(8)-Zn(1)-O(4)	89.77(16)
Zn(1)-O(3)	2.125(4)	O(7)-Zn(1)-O(4)	157.62(16)
Zn(2)-O(6)	2.068(4)	N(5)-Zn(1)-O(4)	97.31(17)
Zn(2)-O(5)	2.095(4)	N(7)-Zn(1)-O(4)	76.36(16)
Zn(2)-N(1)	2.097(5)	O(8)-Zn(1)-O(3)	159.34(16)
Zn(2)-O(1)	2.121(4)	O(7)-Zn(1)-O(3)	92.94(17)
Zn(2)-N(3)	2.124(5)	N(5)-Zn(1)-O(3)	76.30(17)
Zn(2)-O(2)	2.140(5)	N(7)-Zn(1)-O(3)	97.35(16)
O(6)-C(16)	1.349(7)	O(4)-Zn(1)-O(3)	96.13(17)
O(3)-C(25)	1.242(8)	O(6)-Zn(2)-O(5)	89.79(16)
O(4)-C(17)	1.254(7)	O(6)-Zn(2)-N(1)	103.89(18)
O(8)-C(28)	1.342(7)	O(5)-Zn(2)-N(1)	82.67(17)

O(2)-C(9)	1.256(8)	O(6)-Zn(2)-O(1)	94.29(18)
O(1)-C(1)	1.212(8)	O(5)-Zn(2)-O(1)	159.34(17)
O(7)-C(24)	1.352(7)	N(1)-Zn(2)-O(1)	76.69(18)
O(5)-C(7)	1.325(7)	O(6)-Zn(2)-N(3)	83.25(18)
N(7)-C(18)	1.292(7)	O(5)-Zn(2)-N(3)	102.19(17)
N(7)-N(8)	1.379(6)	N(1)-Zn(2)-N(3)	171.50(19)
N(5)-C(26)	1.289(7)	O(1)-Zn(2)-N(3)	98.40(17)
N(5)-N(6)	1.383(7)	O(6)-Zn(2)-O(2)	157.83(18)
N(3)-C(10)	1.268(8)	O(5)-Zn(2)-O(2)	90.27(17)
N(3)-N(4)	1.378(7)	N(1)-Zn(2)-O(2)	98.10(19)
N(8)-C(17)	1.346(7)	O(1)-Zn(2)-O(2)	93.43(17)
N(1)-C(2)	1.285(8)	N(3)-Zn(2)-O(2)	75.08(19)
N(1)-N(2)	1.386(7)	C(16)-O(6)-Zn(2)	132.0(4)
C(18)-C(19)	1.437(8)	C(25)-O(3)-Zn(1)	114.0(4)
C(19)-C(20)	1.404(8)	C(17)-O(4)-Zn(1)	114.0(4)
C(19)-C(24)	1.408(8)	C(28)-O(8)-Zn(1)	131.9(4)
C(31)-C(32)	1.377(9)	C(9)-O(2)-Zn(2)	113.1(4)
C(31)-C(30)	1.382(9)	C(1)-O(1)-Zn(2)	113.8(4)
C(23)-C(22)	1.374(9)	C(24)-O(7)-Zn(1)	132.5(3)
C(23)-C(24)	1.397(8)	C(7)-O(5)-Zn(2)	133.0(3)
C(17)-C(40)	1.495(8)	C(18)-N(7)-N(8)	116.3(4)
C(21)-C(20)	1.390(9)	C(18)-N(7)-Zn(1)	132.1(4)
C(21)-C(22)	1.397(9)	N(8)-N(7)-Zn(1)	111.5(3)
C(26)-C(27)	1.445(8)	C(26)-N(5)-N(6)	117.0(5)
C(2)-C(3)	1.451(8)	C(26)-N(5)-Zn(1)	131.4(4)
N(6)-C(25)	1.340(8)	N(6)-N(5)-Zn(1)	111.6(3)
C(29)-C(30)	1.378(8)	C(10)-N(3)-N(4)	117.7(5)
C(29)-C(28)	1.410(8)	C(10)-N(3)-Zn(2)	130.4(4)
N(2)-C(1)	1.362(8)	N(4)-N(3)-Zn(2)	111.8(4)
C(8)-C(4)	1.389(9)	C(17)-N(8)-N(7)	116.7(4)
C(8)-C(5)	1.389(9)	C(2)-N(1)-N(2)	116.2(5)
C(6)-C(5)	1.386(8)	C(2)-N(1)-Zn(2)	132.4(4)
C(6)-C(7)	1.397(8)	N(2)-N(1)-Zn(2)	111.4(4)
C(15)-C(14)	1.378(9)	N(7)-C(18)-C(19)	123.9(5)
C(15)-C(16)	1.389(9)	C(20)-C(19)-C(24)	118.3(5)
C(27)-C(28)	1.405(8)	C(20)-C(19)-C(18)	116.7(5)
C(27)-C(32)	1.406(8)	C(24)-C(19)-C(18)	124.9(5)
N(4)-C(9)	1.312(9)	C(32)-C(31)-C(30)	120.0(6)
C(13)-C(12)	1.354(10)	C(22)-C(23)-C(24)	121.0(6)
C(13)-C(14)	1.394(9)	O(4)-C(17)-N(8)	121.0(5)
C(11)-C(16)	1.419(8)	O(4)-C(17)-C(40)	123.1(5)
C(11)-C(12)	1.422(9)	N(8)-C(17)-C(40)	115.9(5)
C(11)-C(10)	1.437(8)	C(20)-C(21)-C(22)	118.5(5)
C(7)-C(3)	1.425(8)	N(5)-C(26)-C(27)	124.3(5)
C(9)-C(35)	1.508(9)	N(1)-C(2)-C(3)	124.2(6)
C(25)-C(48)	1.524(9)	C(25)-N(6)-N(5)	116.7(5)
C(3)-C(4)	1.406(8)	C(30)-C(29)-C(28)	121.4(6)
C(1)-C(45)	1.515(9)	C(1)-N(2)-N(1)	115.5(5)
C(41)-C(42)	1.501(10)	C(4)-C(8)-C(5)	118.9(6)
C(41)-C(40)	1.542(8)	C(5)-C(6)-C(7)	121.6(6)
O(10)-C(39)	1.415(10)	C(14)-C(15)-C(16)	121.9(6)
C(42)-C(43)	1.554(10)	C(28)-C(27)-C(32)	119.0(5)
C(35)-C(36)	1.542(10)	C(28)-C(27)-C(26)	124.5(5)
O(11)-C(44)	1.394(10)	C(32)-C(27)-C(26)	116.5(5)
C(45)-C(46)	1.569(12)	C(9)-N(4)-N(3)	116.7(5)
C(43)-C(44)	1.483(12)	C(12)-C(13)-C(14)	118.9(6)
C(38)-C(39)	1.505(11)	O(8)-C(28)-C(27)	122.3(5)
C(38)-C(37)	1.525(11)	O(8)-C(28)-C(29)	119.3(5)
C(49)-C(50)	1.537(11)	C(27)-C(28)-C(29)	118.4(5)
C(49)-C(48)	1.598(14)	O(7)-C(24)-C(23)	118.9(5)
C(46)-C(47)	1.499(11)	O(7)-C(24)-C(19)	121.6(5)
C(36)-C(37)	1.532(10)	C(23)-C(24)-C(19)	119.5(5)
C(47)-C(53)	1.518(12)	C(16)-C(11)-C(12)	117.2(6)

O(12)-C(52)	1.390(10)	C(16)-C(11)-C(10)	124.4(6)
O(13)-C(54)	1.538(13)	C(12)-C(11)-C(10)	118.2(5)
C(51)-C(52)	1.537(15)	O(5)-C(7)-C(6)	120.8(5)
C(51)-C(50)	1.541(14)	O(5)-C(7)-C(3)	121.2(5)
C(53)-C(54)	1.490(13)	C(6)-C(7)-C(3)	118.0(5)
		O(2)-C(9)-N(4)	121.7(6)
		O(2)-C(9)-C(35)	121.1(6)
		N(4)-C(9)-C(35)	117.1(6)
		C(6)-C(5)-C(8)	120.8(6)
		O(3)-C(25)-N(6)	121.3(6)
		O(3)-C(25)-C(48)	121.9(6)
		N(6)-C(25)-C(48)	116.6(6)
		C(31)-C(32)-C(27)	121.2(6)
		C(21)-C(20)-C(19)	121.9(5)
		O(6)-C(16)-C(15)	119.6(5)
		O(6)-C(16)-C(11)	121.6(5)
		C(15)-C(16)-C(11)	118.9(5)
		C(4)-C(3)-C(7)	119.2(5)
		C(4)-C(3)-C(2)	116.6(5)
		C(7)-C(3)-C(2)	124.2(5)
		O(1)-C(1)-N(2)	122.2(6)
		O(1)-C(1)-C(45)	123.9(6)
		N(2)-C(1)-C(45)	113.8(6)
		N(3)-C(10)-C(11)	125.2(5)
		C(29)-C(30)-C(31)	120.0(6)
		C(13)-C(12)-C(11)	123.0(6)
		C(8)-C(4)-C(3)	121.5(6)
		C(23)-C(22)-C(21)	120.7(6)
		C(15)-C(14)-C(13)	120.1(6)
		C(42)-C(41)-C(40)	114.2(5)
		C(17)-C(40)-C(41)	111.2(5)
		C(41)-C(42)-C(43)	111.4(6)
		C(9)-C(35)-C(36)	112.0(6)
		C(1)-C(45)-C(46)	109.9(6)
		C(44)-C(43)-C(42)	114.6(7)
		C(39)-C(38)-C(37)	112.6(6)
		O(10)-C(39)-C(38)	110.0(6)
		O(11)-C(44)-C(43)	112.9(8)
		C(50)-C(49)-C(48)	114.1(7)
		C(47)-C(46)-C(45)	114.0(7)
		C(37)-C(36)-C(35)	113.0(6)
		C(38)-C(37)-C(36)	112.9(6)
		C(25)-C(48)-C(49)	109.9(7)
		C(46)-C(47)-C(53)	114.0(7)
		C(52)-C(51)-C(50)	114.7(8)
		C(49)-C(50)-C(51)	113.5(8)
		C(54)-C(53)-C(47)	115.4(7)
		O(12)-C(52)-C(51)	109.9(8)
		C(53)-C(54)-O(13)	107.7(8)

- *<u>Compound Cu-3a</u>*

DISTANCES		**ANGLES**	
O(6)-N(4)	1.223(2)	O(6)-N(4)-O(5)	122.34(19)
O(5)-N(4)	1.225(2)	O(6)-N(4)-O(4)	118.99(18)
N(4)-O(4)	1.255(2)	O(5)-N(4)-O(4)	118.66(17)
Cu(1)-N(1)	1.9319(14)	N(1)-Cu(1)-O(1)#1	91.80(5)
Cu(1)-O(1)#1	1.9390(11)	N(1)-Cu(1)-O(1)	168.18(6)

Cu(1)-O(1)	1.9627(12)	O(1)#1-Cu(1)-O(1)	80.00(5)
Cu(1)-O(2)	1.9959(13)	N(1)-Cu(1)-O(2)	80.77(5)
Cu(1)-O(4)	2.2465(15)	O(1)#1-Cu(1)-O(2)	165.43(6)
Cu(1)-Cu(1)#1	2.9889(4)	O(1)-Cu(1)-O(2)	105.25(5)
O(2)-C(1)	1.246(2)	N(1)-Cu(1)-O(4)	99.92(6)
O(3)-C(13)	1.426(2)	O(1)#1-Cu(1)-O(4)	109.46(6)
O(1)-C(2)	1.3475(19)	O(1)-Cu(1)-O(4)	90.89(6)
O(1)-Cu(1)#1	1.9391(11)	O(2)-Cu(1)-O(4)	84.29(7)
N(1)-C(8)	1.279(2)	N(1)-Cu(1)-Cu(1)#1	131.54(4)
N(1)-N(2)	1.3835(19)	O(1)#1-Cu(1)-Cu(1)#1	40.29(3)
C(5)-C(6)	1.412(2)	O(1)-Cu(1)-Cu(1)#1	39.71(3)
C(5)-C(2)#1	1.412(2)	O(2)-Cu(1)-Cu(1)#1	143.19(4)
C(5)-C(8)	1.439(2)	O(4)-Cu(1)-Cu(1)#1	103.08(5)
N(2)-C(1)	1.334(2)	C(1)-O(2)-Cu(1)	112.24(11)
C(6)-C(7)	1.370(3)	C(2)-O(1)-Cu(1)#1	127.46(10)
C(2)-C(3)	1.398(2)	C(2)-O(1)-Cu(1)	132.54(10)
C(2)-C(5)#1	1.412(2)	Cu(1)#1-O(1)-Cu(1)	100.00(5)
C(4)-C(3)	1.379(3)	C(8)-N(1)-N(2)	119.43(14)
C(4)-C(7)#1	1.381(3)	C(8)-N(1)-Cu(1)	128.99(12)
C(13)-C(12)	1.507(3)	N(2)-N(1)-Cu(1)	111.57(10)
C(1)-C(9)	1.492(2)	N(4)-O(4)-Cu(1)	120.74(11)
C(9)-C(10)	1.518(2)	C(6)-C(5)-C(2)#1	119.09(16)
C(7)-C(4)#1	1.381(3)	C(6)-C(5)-C(8)	116.12(16)
C(11)-C(12)	1.517(2)	C(2)#1-C(5)-C(8)	124.78(15)
C(11)-C(10)	1.523(2)	C(1)-N(2)-N(1)	114.91(13)
		N(1)-C(8)-C(5)	123.70(15)
		C(7)-C(6)-C(5)	121.80(17)
		O(1)-C(2)-C(3)	119.55(15)
		O(1)-C(2)-C(5)#1	122.56(14)
		C(3)-C(2)-C(5)#1	117.89(15)
		C(3)-C(4)-C(7)#1	121.23(18)
		O(3)-C(13)-C(12)	110.30(15)
		C(4)-C(3)-C(2)	121.32(17)
		O(2)-C(1)-N(2)	119.99(15)
		O(2)-C(1)-C(9)	122.68(16)
		N(2)-C(1)-C(9)	117.34(15)
		C(1)-C(9)-C(10)	113.74(15)
		C(6)-C(7)-C(4)#1	118.64(17)
		C(12)-C(11)-C(10)	112.73(15)
		C(9)-C(10)-C(11)	110.94(15)
		C(13)-C(12)-C(11)	113.62(16)
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1			

- *Compound Cu-3b*

DISTANCES		**ANGLES**	
O(3)-C(12)	1.345(6)	C(12)-C(11)-C(10)	114.2(4)
C(11)-C(12)	1.501(5)	O(3)-C(12)-C(11)	110.9(4)
C(11)-C(10)	1.505(5)	C(3)-C(13)-C(4)	118.5(3)
C(13)-C(3)	1.367(5)	O(1)-Cu(1)-N(1)	92.21(10)
C(13)-C(4)	1.386(6)	O(1)-Cu(1)-O(2)	173.02(9)
Cu(1)-O(1)	1.927(2)	N(1)-Cu(1)-O(2)	80.81(10)
Cu(1)-N(1)	1.943(3)	O(1)-Cu(1)-O(1)#1	82.50(9)
Cu(1)-O(2)	1.958(2)	N(1)-Cu(1)-O(1)#1	174.71(10)
Cu(1)-O(1)#1	1.964(2)	O(2)-Cu(1)-O(1)#1	104.47(9)
Cu(1)-Cu(1)#1	2.9261(8)	O(1)-Cu(1)-Cu(1)#1	41.73(6)
O(1)-C(1)	1.335(4)	N(1)-Cu(1)-Cu(1)#1	133.94(8)
O(1)-Cu(1)#1	1.964(2)	O(2)-Cu(1)-Cu(1)#1	145.25(7)

O(2)-C(7)	1.253(4)	O(1)#1-Cu(1)-Cu(1)#1	40.77(6)
N(1)-C(6)	1.278(4)	C(1)-O(1)-Cu(1)	128.0(2)
N(1)-N(2)	1.389(4)	C(1)-O(1)-Cu(1)#1	134.5(2)
C(7)-N(2)	1.321(4)	Cu(1)-O(1)-Cu(1)#1	97.50(9)
C(7)-C(8)	1.497(4)	C(7)-O(2)-Cu(1)	113.8(2)
C(6)-C(2)	1.435(5)	C(6)-N(1)-N(2)	120.3(3)
C(1)-C(5)	1.391(5)	C(6)-N(1)-Cu(1)	128.7(2)
C(1)-C(2)	1.419(5)	N(2)-N(1)-Cu(1)	111.0(2)
C(9)-C(8)	1.515(5)	O(2)-C(7)-N(2)	119.2(3)
C(9)-C(10)	1.517(5)	O(2)-C(7)-C(8)	121.7(3)
C(5)-C(4)	1.377(5)	N(2)-C(7)-C(8)	119.0(3)
C(3)-C(2)	1.414(5)	N(1)-C(6)-C(2)	123.3(3)
Si(1)-F(2)	1.679(2)	C(7)-N(2)-N(1)	115.2(3)
Si(1)-F(2)#2	1.679(2)	O(1)-C(1)-C(5)	120.0(3)
Si(1)-F(1)	1.6854(14)	O(1)-C(1)-C(2)	122.4(3)
Si(1)-F(1)#2	1.6855(14)	C(5)-C(1)-C(2)	117.6(3)
Si(1)-F(1)#3	1.6855(13)	C(8)-C(9)-C(10)	113.0(3)
Si(1)-F(1)#4	1.6855(13)	C(4)-C(5)-C(1)	121.7(3)
		C(7)-C(8)-C(9)	112.5(3)
		C(13)-C(3)-C(2)	121.8(3)
		C(5)-C(4)-C(13)	121.2(3)
		C(3)-C(2)-C(1)	119.1(3)
		C(3)-C(2)-C(6)	115.4(3)
		C(1)-C(2)-C(6)	125.4(3)
		C(11)-C(10)-C(9)	113.7(3)
		F(2)-Si(1)-F(2)#2	180.00(13)
		F(2)-Si(1)-F(1)	90.66(7)
		F(2)#2-Si(1)-F(1)	89.34(7)
		F(2)-Si(1)-F(1)#2	89.34(7)
		F(2)#2-Si(1)-F(1)#2	90.66(7)
		F(1)-Si(1)-F(1)#2	180.0
		F(2)-Si(1)-F(1)#3	89.34(7)
		F(2)#2-Si(1)-F(1)#3	90.66(7)
		F(1)-Si(1)-F(1)#3	91.86(9)
		F(1)#2-Si(1)-F(1)#3	88.13(9)
		F(2)-Si(1)-F(1)#4	90.66(7)
		F(2)#2-Si(1)-F(1)#4	89.34(7)
		F(1)-Si(1)-F(1)#4	88.14(9)
		F(1)#2-Si(1)-F(1)#4	91.87(9)
		F(1)#3-Si(1)-F(1)#4	180.0
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+2 #2 -x+1,-y+1,-z+2 #3 -x+1,y,-z+2 #4 x,-y+1,z			

- *Compound Ni-3a*

DISTANCES		ANGLES	
Ni(1)-N(1)#1	1.985(5)	N(1)#1-Ni(1)-O(1)	171.37(17)
Ni(1)-O(1)#1	2.017(4)	O(1)#1-Ni(1)-O(1)	81.58(17)
Ni(1)-O(1)	2.034(4)	N(1)#1-Ni(1)-O(2)#1	78.45(17)
Ni(1)-O(2)#1	2.082(4)	O(1)#1-Ni(1)-O(2)#1	168.17(16)
Ni(1)-O(4)	2.120(5)	O(1)-Ni(1)-O(2)#1	110.13(17)
Ni(1)-O(3)	2.137(5)	N(1)#1-Ni(1)-O(4)	94.1(2)
O(1)-C(1)	1.321(6)	O(1)#1-Ni(1)-O(4)	91.49(18)
O(1)-Ni(1)#1	2.017(4)	O(1)-Ni(1)-O(4)	86.81(19)
O(2)-C(8)	1.236(7)	O(2)#1-Ni(1)-O(4)	90.88(19)
O(2)-Ni(1)#1	2.082(4)	N(1)#1-Ni(1)-O(3)	91.89(19)
O(3)-C(20)	1.434(9)	O(1)#1-Ni(1)-O(3)	86.82(19)
N(1)-C(7)	1.271(7)	O(1)-Ni(1)-O(3)	87.02(17)
N(1)-N(2)	1.384(6)	O(2)#1-Ni(1)-O(3)	91.99(19)

N(1)-Ni(1)#1	1.985(5)	O(4)-Ni(1)-O(3)	173.78(19)
N(2)-C(8)	1.334(8)	C(1)-O(1)-Ni(1)#1	128.4(3)
C(1)-C(2)	1.400(8)	C(1)-O(1)-Ni(1)	132.9(3)
C(1)-C(6)	1.421(7)	Ni(1)#1-O(1)-Ni(1)	98.42(16)
C(2)-C(3)	1.374(8)	C(8)-O(2)-Ni(1)#1	112.8(4)
C(3)-C(4)	1.392(9)	C(20)-O(3)-Ni(1)	122.4(5)
C(4)-C(5)	1.377(9)	C(7)-N(1)-N(2)	118.9(5)
C(5)-C(6)	1.385(8)	C(7)-N(1)-Ni(1)#1	128.7(4)
C(6)-C(7)	1.443(8)	N(2)-N(1)-Ni(1)#1	112.2(4)
C(8)-C(9)	1.484(8)	C(8)-N(2)-N(1)	116.5(5)
O(10)-N(10)	1.257(7)	O(1)-C(1)-C(2)	119.7(5)
O(5)-C(13)	1.370(9)	O(1)-C(1)-C(6)	122.7(5)
O(11)-N(10)	1.231(7)	C(2)-C(1)-C(6)	117.5(5)
N(10)-O(12)	1.247(8)	C(3)-C(2)-C(1)	120.9(5)
C(9)-C(10)	1.520(11)	C(2)-C(3)-C(4)	121.9(6)
C(13)-C(12)	1.527(9)	C(5)-C(4)-C(3)	117.5(6)
C(10)-C(11)	1.532(10)	C(4)-C(5)-C(6)	122.5(6)
C(11)-C(12)	1.405(12)	C(5)-C(6)-C(1)	119.7(5)
C(20)-C(21)	1.452(11)	C(5)-C(6)-C(7)	115.4(5)
		C(1)-C(6)-C(7)	124.9(5)
		N(1)-C(7)-C(6)	125.1(5)
		O(2)-C(8)-N(2)	119.9(5)
		O(2)-C(8)-C(9)	123.0(6)
		N(2)-C(8)-C(9)	117.0(5)
		O(11)-N(10)-O(12)	123.2(6)
		O(11)-N(10)-O(10)	121.3(6)
		O(12)-N(10)-O(10)	115.5(6)
		C(8)-C(9)-C(10)	112.9(6)
		O(5)-C(13)-C(12)	108.6(6)
		C(9)-C(10)-C(11)	115.0(7)
		C(12)-C(11)-C(10)	114.7(8)
		C(11)-C(12)-C(13)	114.8(7)
		O(3)-C(20)-C(21)	112.7(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z

- *Compound NiL**

DISTANCES		**ANGLES**	
Ni(1)-O(10)#1	1.842(4)	O(10)#1-Ni(1)-O(10)	180.0
Ni(1)-O(10)	1.842(4)	O(10)#1-Ni(1)-N(2)	96.39(19)
Ni(1)-N(2)	1.901(5)	O(10)-Ni(1)-N(2)	83.61(19)
Ni(1)-N(2)#1	1.901(5)	O(10)#1-Ni(1)-N(2)#1	83.60(19)
N(2)-C(14)	1.238(7)	O(10)-Ni(1)-N(2)#1	96.39(19)
N(2)-N(1)	1.407(6)	N(2)-Ni(1)-N(2)#1	180.00(16)
O(10)-C(7)	1.271(6)	C(14)-N(2)-N(1)	122.6(5)
C(3)-C(4)	1.362(8)	C(14)-N(2)-Ni(1)	125.2(5)
C(3)-C(2)	1.386(7)	N(1)-N(2)-Ni(1)	112.2(3)
C(2)-C(1)	1.365(8)	C(7)-O(10)-Ni(1)	110.7(4)
C(1)-C(6)	1.359(9)	C(4)-C(3)-C(2)	119.2(6)
C(1)-C(7)	1.542(8)	C(1)-C(2)-C(3)	122.6(6)
C(7)-N(1)	1.304(6)	C(6)-C(1)-C(2)	117.5(6)
C(6)-C(5)	1.395(9)	C(6)-C(1)-C(7)	120.9(5)
C(4)-O(11)	1.379(7)	C(2)-C(1)-C(7)	121.6(5)
C(4)-C(5)	1.395(10)	O(10)-C(7)-N(1)	125.4(5)
O(12)-C(11)	1.366(6)	O(10)-C(7)-C(1)	115.7(5)
C(11)-C(12)	1.370(8)	N(1)-C(7)-C(1)	118.9(5)
C(11)-C(10)	1.394(7)	C(1)-C(6)-C(5)	122.2(6)

C(10)-C(9)	1.375(7)	C(3)-C(4)-O(11)	122.2(6)
C(8)-C(13)	1.399(8)	C(3)-C(4)-C(5)	119.7(6)
C(8)-C(9)	1.402(8)	O(11)-C(4)-C(5)	118.1(6)
C(8)-C(14)	1.479(8)	C(6)-C(5)-C(4)	118.7(6)
C(12)-C(13)	1.373(9)	C(7)-N(1)-N(2)	108.0(4)
C(21)-C(20)	1.298(19)	O(12)-C(11)-C(12)	118.3(5)
C(21)-C(21)#2	1.41(2)	O(12)-C(11)-C(10)	120.8(5)
O(1)-C(20)	1.363(18)	C(12)-C(11)-C(10)	120.9(5)
O(1)-C(20)#2	1.363(18)	C(9)-C(10)-C(11)	119.6(5)
		C(13)-C(8)-C(9)	118.4(5)
		C(13)-C(8)-C(14)	113.2(6)
		C(9)-C(8)-C(14)	128.4(6)
		C(10)-C(9)-C(8)	120.4(5)
		N(2)-C(14)-C(8)	129.7(6)
		C(11)-C(12)-C(13)	119.5(6)
		C(12)-C(13)-C(8)	121.1(6)
		C(20)-C(21)-C(21)#2	106.7(11)
		C(20)-O(1)-C(20)#2	107(2)
		C(21)-C(20)-O(1)	108.4(19)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+3/2,-z+1 #2 -x+1,y,-z+1/2

Table S3. Main hydrogen bonds (Å) and angles (°).

D–H···A	D–H	H···A	D···A	D–H···A
H_2L				
O(2)-H(1)...O(1)#1	0.75(4)	2.06(4)	2.797(3)	167(4)
N(2)-H(2)...O(1)#2	0.68(4)	2.24(4)	2.923(2)	176(3)
C(1)-H(7)...O(2)#3	0.94(3)	2.64(3)	3.504(3)	152(2)
O(3)-H(3)...N(1)	0.82	1.94	2.613(3)	138.3
O(3)-H(3)...N(1)	0.82	1.94	2.613(3)	138.3
C(1)-H(7)...O(2)#3	0.94(3)	2.64(3)	3.504(3)	152(2)
N(2)-H(2)...O(1)#2	0.68(4)	2.24(4)	2.923(2)	176(3)
O(2)-H(1)...O(1)#1	0.75(4)	2.06(4)	2.797(3)	167(4)
#1= -x+1,-y+2,-z+1 #2= -x,-y+1,-z+1 #3= x-1,y-1,z				
Compound Zn-1a				
O8-H7…O5#1	0.96(8)	1.47(8)	2.424(7)	173(10)
O10-H10A...O #2	0.84	1.95	2.757(8)	161
O11-H11...O4 #3	0.84	2.03	2.804(10)	153
O12-H12A...O53 #3	0.84	2.08	2.855(10)	153
O15-H15…O56 #3	0.84	2.07	2.772(9)	140
N2-H30 ...O53	0.79(9)	1.96(9)	2.751(9)	175(11)
O40-H40…O52 #4	0.84	2.01	2.779(9)	152
N4-H41…O40 #5	0.97(9)	1.84(9)	2.789(8	167(5)
N6-H61…O54.	0.80(9).	1.99(9)	2.777(9)	168(9)
O6-H601…O7 #6	0.92(8)	1.52(8)	2.431(7)	171(9)
N8-H801…O15 #3	1.04(8	1.72(8)	2.752(7)	169(4)
#1= 1+x,y,z; #2=-x,-y,1-z; #3=1-x,-y,-z #4=1-x,1-y,1-z; #5=-x,1-y,1-z; #6=-1+x,y,z				
Compound Cu-3a				
N2-H2...O3#1	0.86	1.90	2.742(2)	168
O3 -H3…O4#2	0.82	1.92	2.732(2)	174
#1 = 2-x,1/2+y,1/2-z, #2 =1+x,1/2-y,1/2+z				
Compound Cu-3b				
O3-H3…F2#1	0.82	2.34	2.881(5)	124
N2-H6…F2 #2	0.86	1.96	2.792(4)	161
#1 =1/2-x,1/2+y,1-z #2 =1/2+x,1/2+y,z				
Compound Ni-3a				
N2-H1…O11 #1	0.91(6)	2.00(7)	2.909(7)	178(7)
O4-H4WA…O5 #2	0.66(7)	2.06(7)	2.694(8)	163(8)
O4-H4WB…O10 #3	0.78(9)	2.05(9)	2.777(8)	154(9)
O5-H5A…O10	0.82	1.96	2.761(9)	167
O3-H101…O1 #4	0.70(8)	2.53(8)	2.856(7)	112(8)
O3-H101…O4 #4	0.70(8)	2.28(8)	2.877(8)	144(8)
#1 = -x,1-y,1-z ; #2 = 1-x,1-y,2-z ; #3 = x,-1+y,1+z; #4 =1-x,-y,2-z				

Compound NiL*				
O11 -H11…O20 #1	0.82	2.16	2.947(10)	162
O12 -H12...O12 #2	0.82	2.06	2.731(6)	139

#1= 1/2-x,-1/2+y,1/2-z ; #2=x,-y,-z

Figure S1. Diffuse reflectance spectra of **[$Cu_2(HL)_2(SiF_6)$] (Cu-3b)** (blue) y **[Cu(L)] (Cu-5)** (red) and free ligand (**H_2L**) (grey**)**

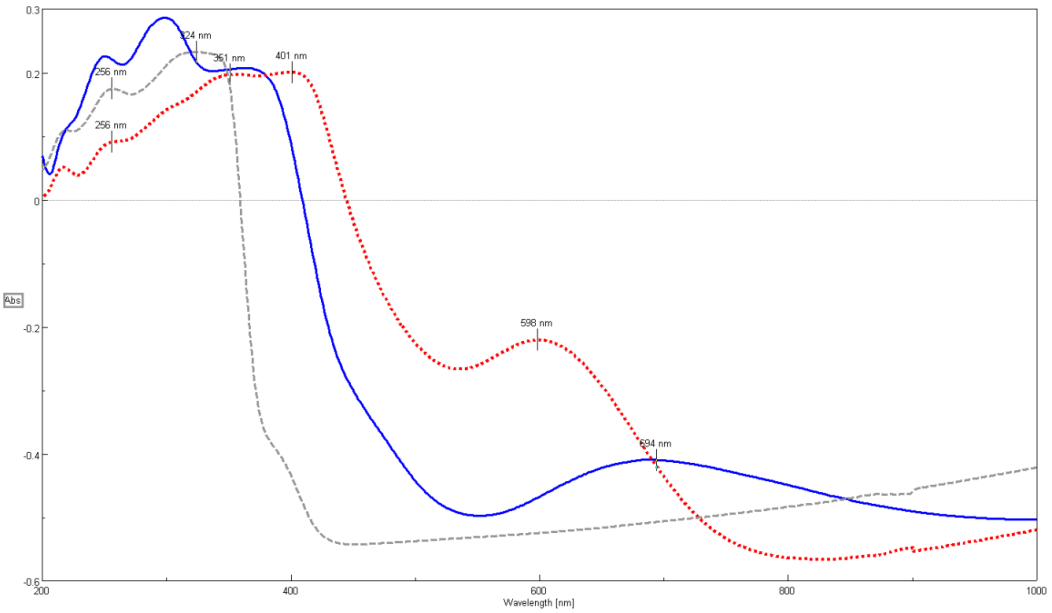

Figure S2. Diffuse reflectance spectra of **[Ni(HL)$_2$] (Ni-2)** (blue) and **[Ni(L)] (Ni-5)** (red) and free ligand (**H_2L**) (grey**)**

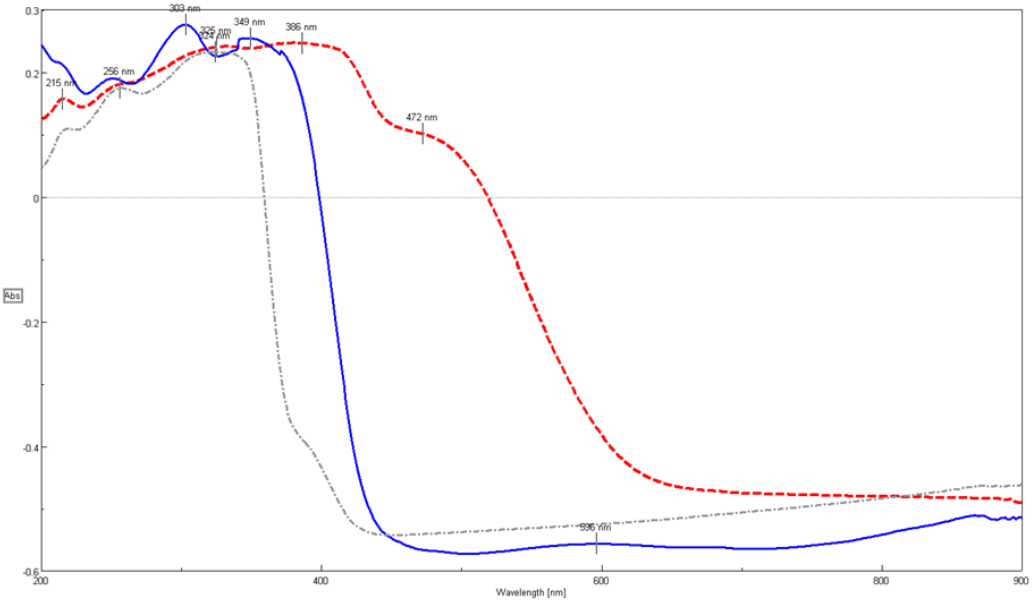

Figure S3. Diffuse reflectance spectra of **[Cu(L)] (Cu-5)** (blue) and **[Ni(L)] (Ni-5)** (red)

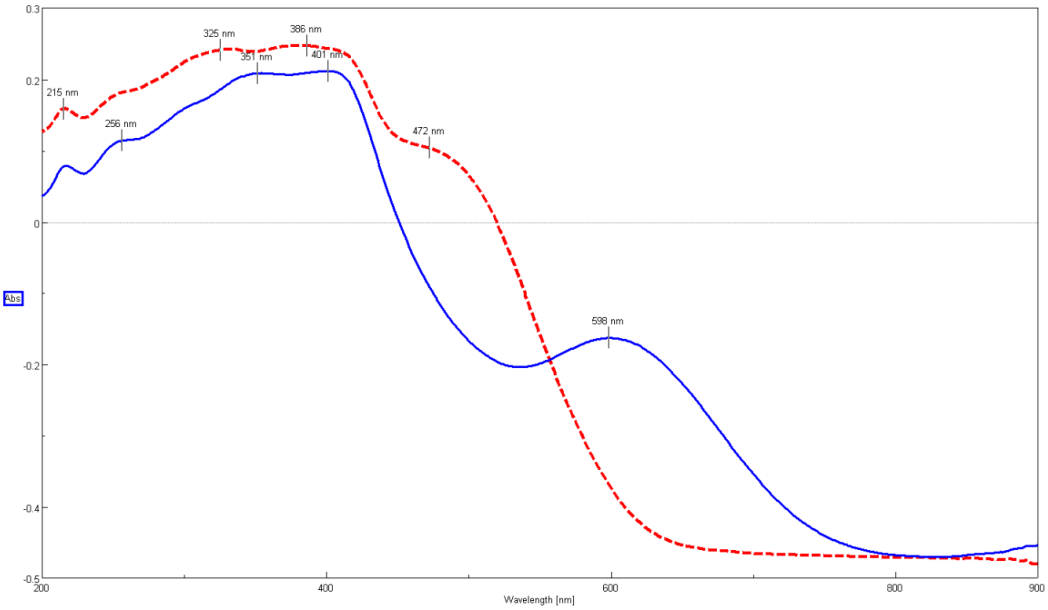

Table S4. UV-vis absorption bands of the compounds in solid state and ethanol solution

Compound	λ (nm)	
	Solid	Solution
H_2L	324, 256	322, 288, 278, 217
$[Cu_2(HL)]_2(NO_3)_2]$ *(Cu-3a)*	699; 377, 256, 213	689; 390, 283, 205
$[Cu_2(HL)_2(SiF_6)]$ *(Cu-3b)*	697; 377, 256	
Cu(L) *(Cu-5)*	598 , 401, 351, 256	376, 312, 295, 259, 230, 286,
$[Ni(HL)_2]$ *(Ni-2)*	948 , 596 349, 303, 248	409, 353, 289, 236
$[Ni_2(HL)]_2(NO_3)_2]$ *(Ni-3)*	946 ,592, 303	
Ni(L) *(Ni-5)*	468 383, 345, 246	596, 388, 322, 288, 221
$[Zn(HL)_2]$ *(Zn-2)*	385, 268	375, 295, 288, 250
$[Zn_2(HL)]_2(NO_3)_2$ *(Zn-3)*	403, 371, 306	385, 298, 288, 250, 232
$[Zn_2L_2]$ *(Zn-4)*	407, 368, 306	373, 353, 295, 251, 226

Figure S4. Experimental X-ray powder diffraction of **Cu-5** (red), **Ni-5** (green) compared with the one calculated from single crystals of Cu-5 (blue) [9].