Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Fe^{II}, Co^{II} and Ni^{II} complexes based on 1-chloro-3-(pyridin-2-yl)imidazo[1,5-a]pyridine: synthesis, structures, single-molecule magnetic and electrocatalytic properties

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Content

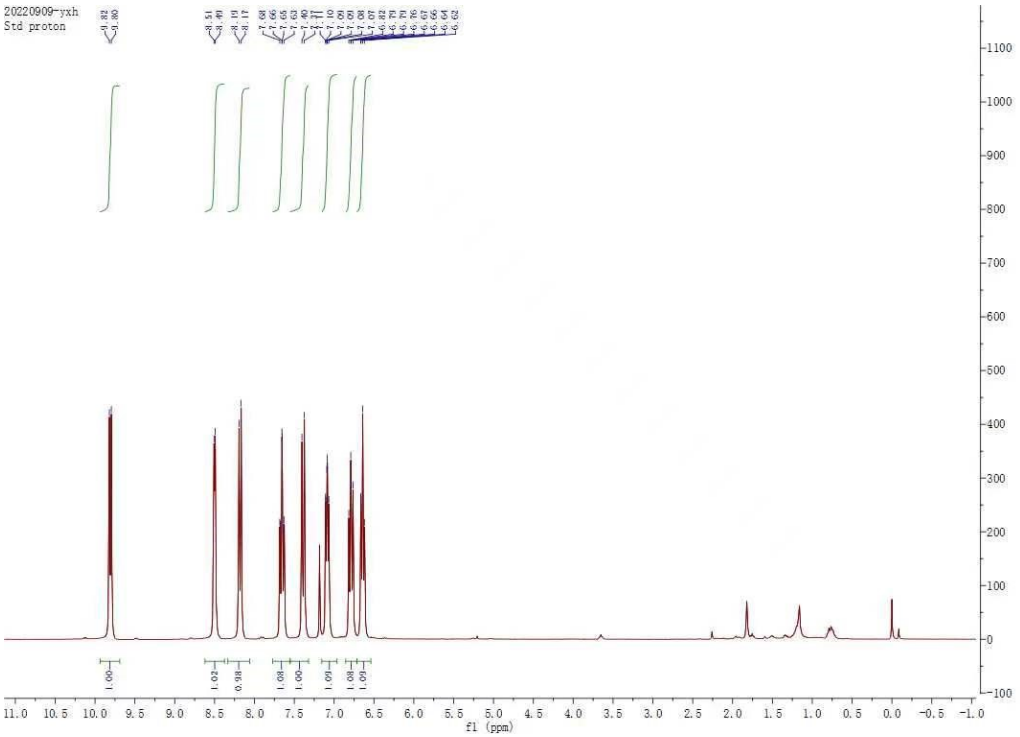


Figure S1 ^{1}H NMR spectrum of the L ligand.

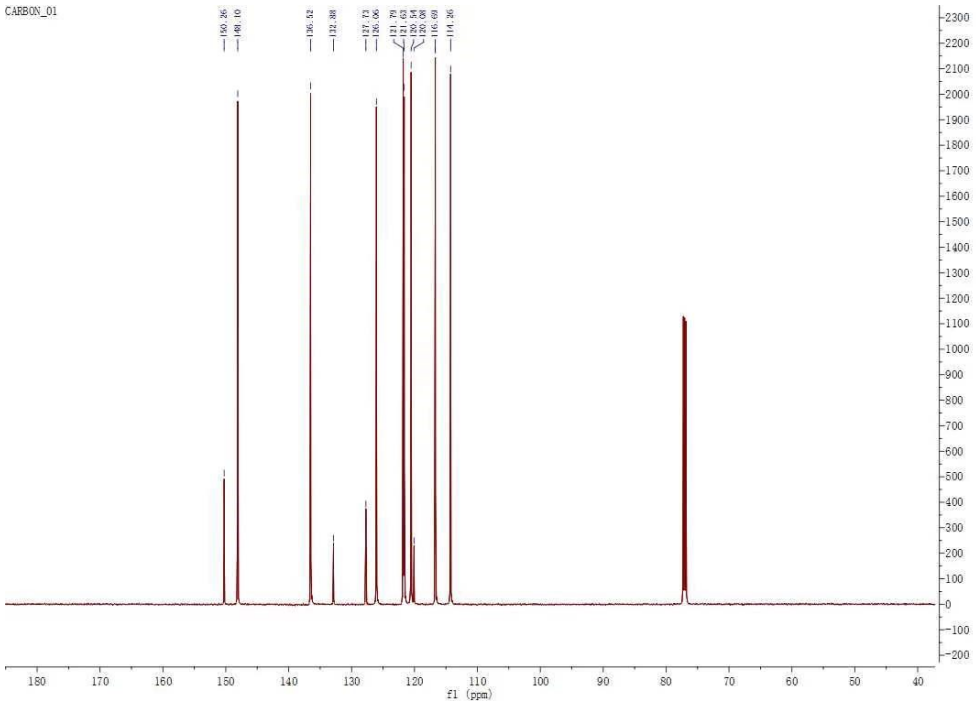


Figure S2 ^{13}C NMR spectrum of the L ligand.

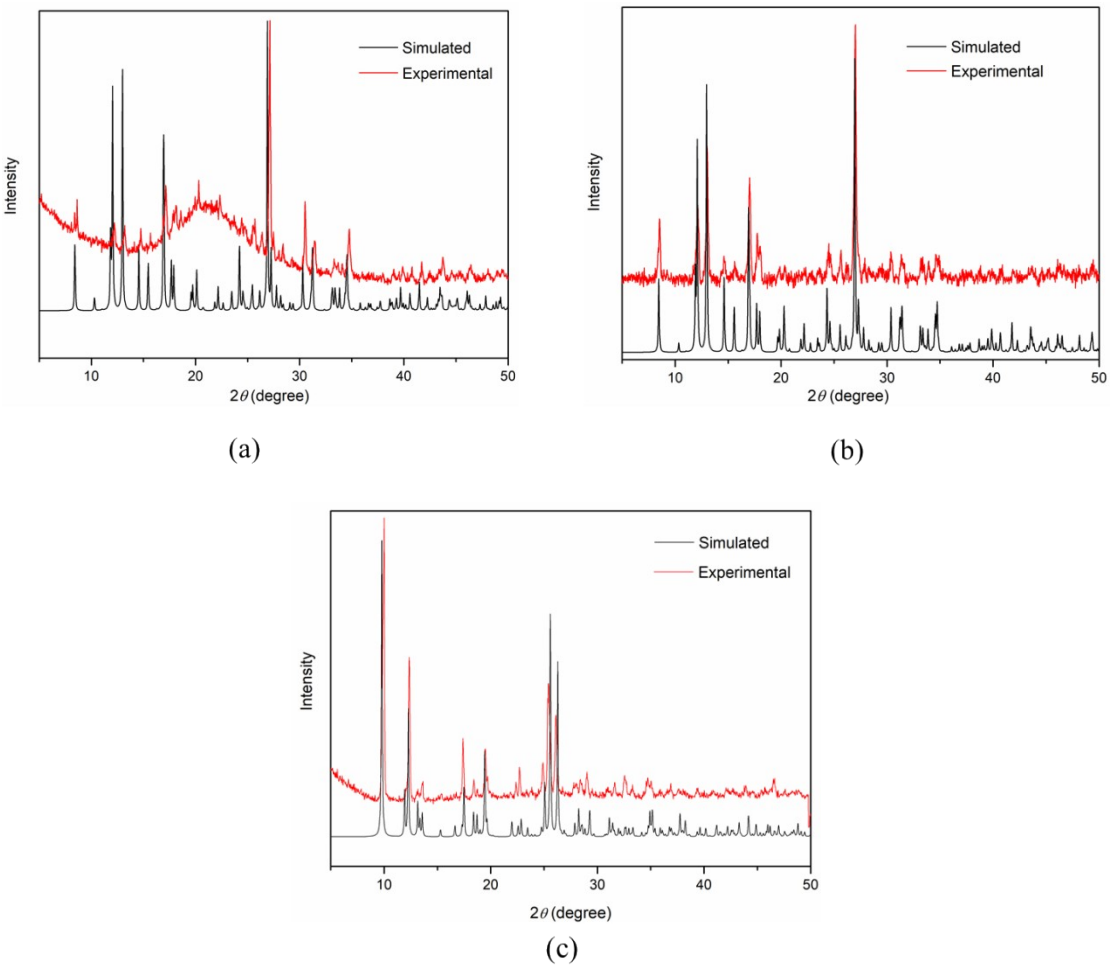
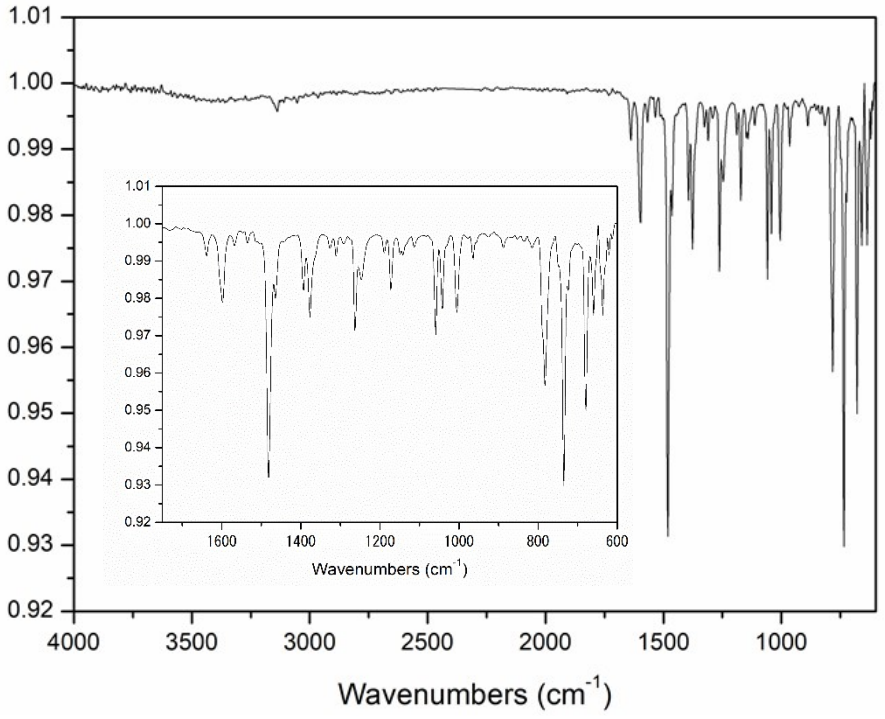


Figure S3 PXRD patterns of complexes **1**(a), **2**(b) and **3**(c).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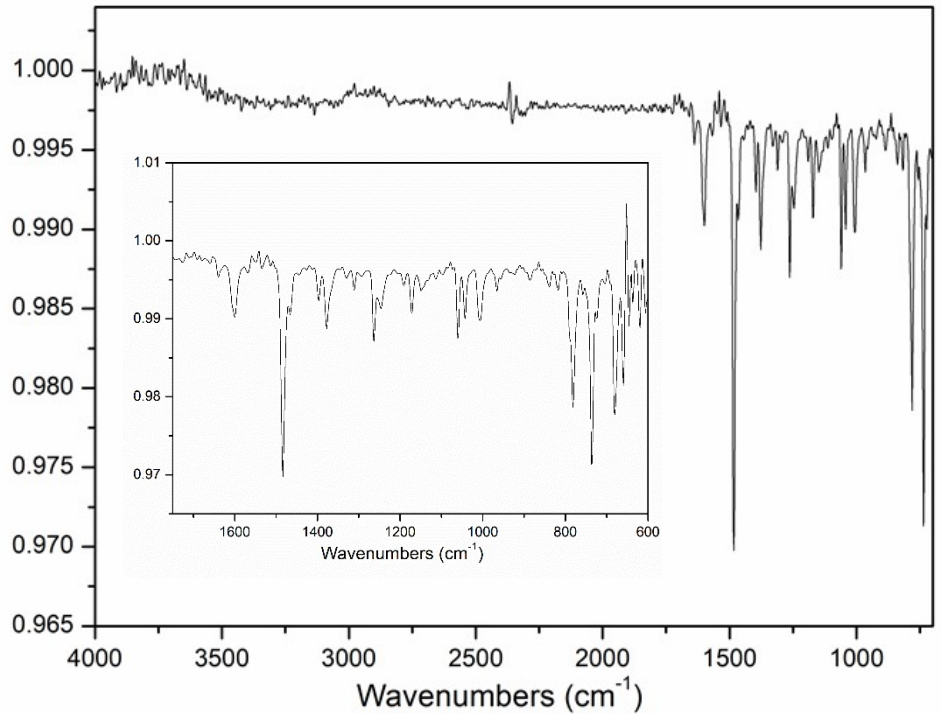
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
4000
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

(a)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0.990
0.985
0.980
0.975
0.970
0.965
4000
3500
3000
2500
2000
1500
1000
Wavenumbers (cm-1)
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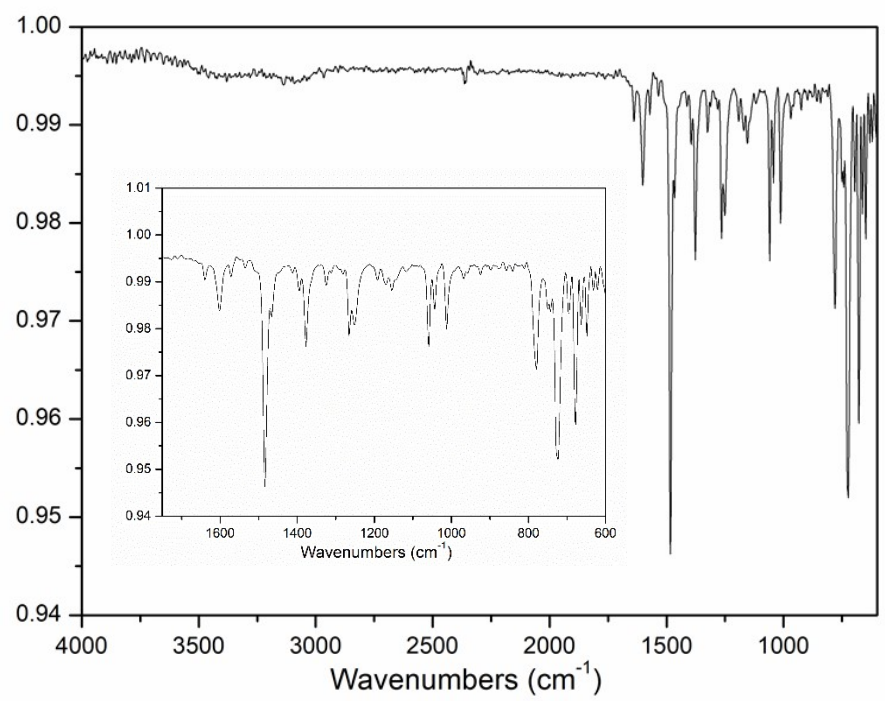
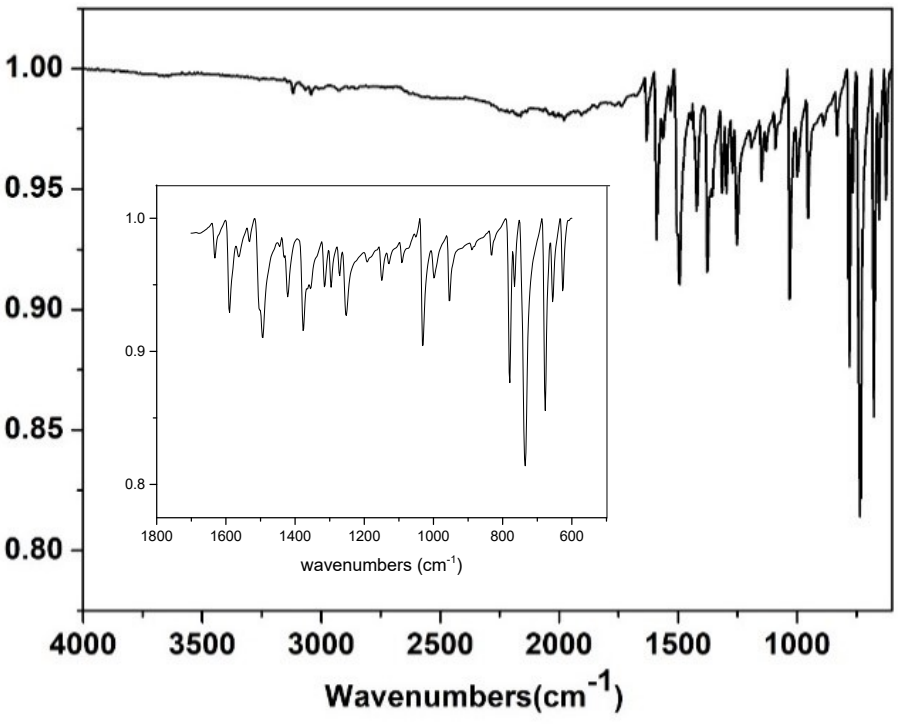
1.00
0.99
0.98
0.97
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

(b)



(c)



(d)

Figure S4 FT-IR spectra of complexes **1**(a), **2**(b) and **3**(c) and the L ligand (d).

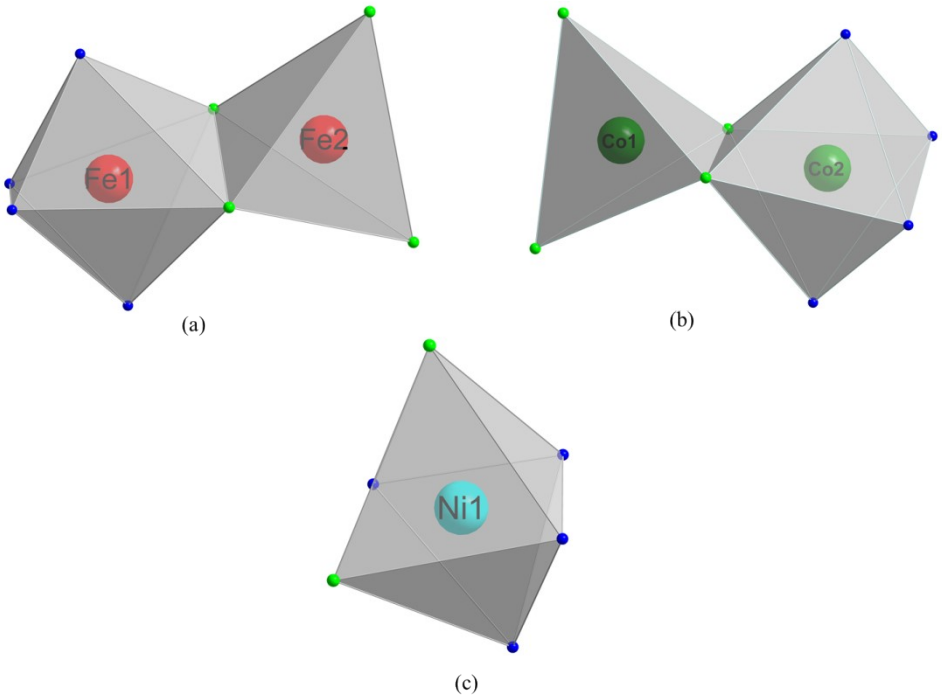


Figure S5 Coordination environments of metals of complexes **1**(a), **2**(b) and **3**(c).

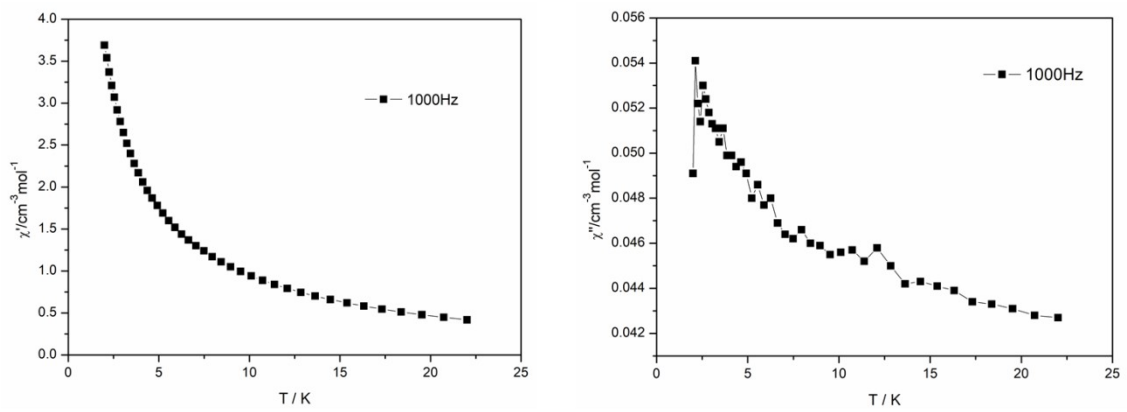


Figure S6 Temperature dependence of the in-phase χ' (a) and out-of-phase χ'' (b) susceptibilities for complex **1** at zero dc field and the frequency of 1000 Hz between 2 and 22 K.

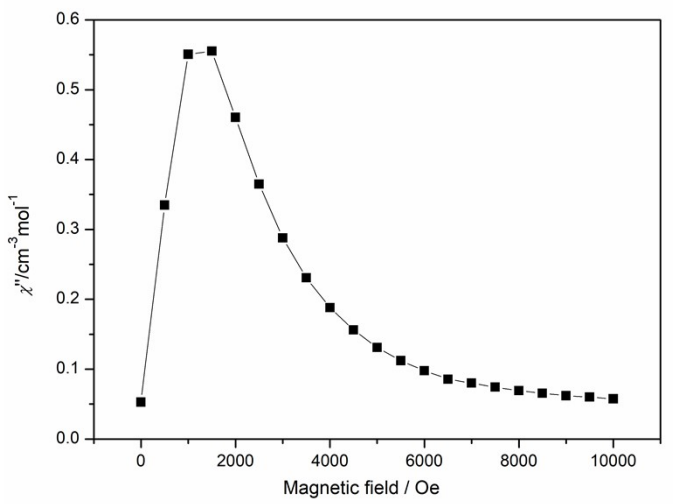


Figure S7 Magnetic field dependence of the out-of-phase (χ'') susceptibilities for **1** in the 0-10000 Oe dc field (at temperature of 2 K and frequency of 1000 Hz).

Table S1 Selected bond lengths (Å) and angles (°) of **1-3**

Compound **1**			
Fe1-Cl4[1]	2.5029(9)	Fe1-Cl4	2.5028(10)
Fe1-N4[1]	2.166(3)	Fe1-N4	2.167(3)
Fe1-N6[1]	2.219(2)	Fe1-N6	2.219(2)
Fe2-Cl4	2.3990(10)	Fe2-Cl4[1]	2.3989(10)
Fe2-Cl6	2.2516(9)	Fe2-Cl6[1]	2.2515(9)
Cl4-Fe1-Cl4[1]	90.98(4)	N4[1]-Fe1-Cl4	90.83(7)
N4[1]-Fe1-Cl4[1]	167.59(7)	N4-Fe1-Cl4[1]	90.83(7)
N4-Fe1-Cl4	167.59(7)	N4[1]-Fe1-N4	90.03(14)
N4[1]-Fe1-N6	102.03(9)	N4[1]-Fe1-N6[1]	75.05(9)
N4-Fe1-N6	75.05(9)	N4-Fe1-N6[1]	102.03(9)
N6[1]-Fe1-Cl4[1]	92.67(7)	N6-Fe1-Cl4[1]	90.15(7)
N6-Fe1-Cl4	92.67(7)	N6[1]-Fe1-Cl4	90.15(7)
N6[1]-Fe1-N6	175.98(14)	Cl4[1]-Fe2-Cl4	96.15 (5)
Cl6[1]-Fe2-Cl4[1]	108.05 (4)	Cl6-Fe2-Cl4[1]	108.49 (3)
Cl6-Fe2-Cl4	108.05(4)	Cl6[1]-Fe2-Cl4	108.50(3)
Cl6[1]-Fe2-Cl6	124.04(6)	Fe2-Cl4-Fe1	86.44(3)
C14-N4-Fe1	114.6(2)	C17-N4-Fe1	137.1(2)
Compound **2**			
Co1-Cl[1]	2.2338(11)	Co1-Cl1	2.2338(11)
Co1-Cl2	2.3356(12)	Co1-Cl2[1]	2.3356(12)
Co2-Cl2	2.4972(12)	Co2-Cl2[1]	2.4973(12)
Co2-N1[1]	2.171(3)	Co2-N1	2.171(3)
Co2-N2[1]	2.111(3)	Co2-N2	2.111(3)
Cl1[1]-Co1-Cl1	118.26(7)	Cl1[1]-Co1-Cl2	109.07(4)
Cl1[1]-Co1-Cl2[1]	110.22(4)	Cl1-Co1-Cl2[1]	109.07(4)
Cl1-Co1-Cl2	110.23(4)	N1-Co2-Cl2	92.49(9)

N1[1]-Co2-Cl2	88.59(9)	N1-Co2-Cl2[1]	88.59(9)
N1[1]-Co2-Cl2[1]	92.49(9)	N1[1]-Co2-N1	178.48(19)
N2-Co2-Cl2[1]	90.75(9)	N2[1]-Co2-Cl2[1]	169.01(7)
N2-Co2-Cl2	169.01(7)	N2[1]-Co2-Cl2	90.75(9)
N2-Co2-N1	76.55(11)	N2[1]-Co2-N1	102.35(11)
N2-Co2-N1[1]	102.35(11)	N2[1]-Co2-N1[1]	76.55(11)
N2[1]-Co2-N2	90.70(18)	Co1-Cl2-Co2	85.99(4)
C2-N1-Co2	125.3(3)	C5-N1-Co2	116.3(2)
Compound **3**			
Ni1-Cl2	2.4119(5)	Ni1-Cl2[1]	2.4119(6)
Ni1-N2[1]	2.1272(16)	Ni1-N2	2.1272(17)
Ni1-N4	2.0963(16)	Ni1-N4[1]	2.0963(16)
Cl2[1]-Ni1-Cl	294.36(3)	N2[1]-Ni1-Cl2[1]	170.68(5)
N2[1]-Ni1-Cl	291.00(5)	N2-Ni1-Cl2	170.68(5)
N2-Ni1-Cl2[1]	91.00(5)	N2[1]-Ni1-N2	84.74(9)
N4[1]-Ni1-Cl2[1]	94.34(5)	N4-Ni1-Cl2	94.34(5)
N4-Ni1-Cl2[1]	90.64(5)	N4[1]-Ni1-Cl2	90.64(5)
N4[1]-Ni1-N2	96.56(6)	N4[1]-Ni1-N2[1]	77.96(6)
N4-Ni1-N2	77.96(6)	N4-Ni1-N2[1]	96.56(6)
N4-Ni1-N4[1]	172.68(9)	C4-N2-Ni1	111.84(12)
C12-N2-Ni1	140.64(14)	C2-N4-Ni1	116.88(13)

The symmetric code for **1**: [1]1-x,+y,3/2-z; **2**: [1]1-x,+y,3/2-z; **3**: [1]1-x,+y,1/2-z

Table S2 Shape analysis for six-coordinated Fe^{II} ion of complex **1**

HP-6	1	D_{6h}	Hexagon
PPY-6	2	C_{5v}	Pentagonal pyramid
OC-6	3	O_h	Octahedron
TPR-6	4	D_{3h}	Trigonal prism
JPPY-6	5	C_{5v}	Johnson pentagonal pyramid (J2)

Structure [ML_6]	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-6
Complex **1**	28.875	23.710	**1.683**	13.570	28.193

Table S3 Shape analysis for four-coordinated Fe^{II} ion of complex 1

SP-4	1	D_{4h}	Square
T-4	2	Td	Tetrahedron
SS-4	3	C_{2V}	Seesaw

Structure [ML_4]	SP-4	**T-4**	SS-4
Complex **1**	33.445	**0.473**	7.167

Table S4 Shape analysis for six-coordinated Co^{II} ion of complex **2**

HP-6	1	D_{6h}	Hexagon
PPY-6	2	C_{5v}	Pentagonal pyramid
OC-6	3	O_h	Octahedron
TPR-6	4	D_{3h}	Trigonal prism
JPPY-6	5	C_{5v}	Johnson pentagonal pyramid (J2)

Structure [ML_6]	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-6
Complex **2**	28.695	24.026	**1.549**	13.666	28.526

Table S5 Shape analysis for four-coordinated Co^{II} ion of complex 2

SP-4	1	D_{4h}	Square
T-4	2	Td	Tetrahedron
SS-4	3	C_{2V}	Seesaw

Structure [ML_4]	SP-4	**T-4**	SS-4
Complex **2**	32.351	**0.277**	8.388

Table S6 Shape analysis for six-coordinated Ni^{II} ion of complex **3**

HP-6	1	D_{6h}	Hexagon
PPY-6	2	C_{5v}	Pentagonal pyramid
OC-6	3	O_h	Octahedron
TPR-6	4	D_{3h}	Trigonal prism
JPPY-6	5	C_{5v}	Johnson pentagonal pyramid (J2)

Structure [ML_6]	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-6
Complex **3**	29.733	25.386	**1.265**	14.357	30.085