Electronic Supplementary Material (ESI) for CrystEngComm.

Carboxylates *Directed* Versatile Structures of Ten 1D→3D Ni(II) Coordination Polymers: Fluorescent Behaviors and Electrochemical Activities†

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Supporting Information

Table S1 Selected bond distances (Å) and angles (deg) for complex **1**.

1			
Ni(1)–N(1)	2.1044(16)	Ni(1)–N(1)A	2.1045(16)
Ni(1)–O(2)	2.0646(14)	Ni(1)–O(2)A	2.0646(14)
Ni(1)–O(1W)	2.0938(13)	Ni(1)–O(1W)A	2.0938(13)
O(2)–Ni(1)–O(2)A	180.0	O(2)–Ni(1)–N(1)	90.42(6)
O(2)–Ni(1)–O(1W)A	90.54(6)	O(2)A–Ni(1)–N(1)	89.58(6)
O(2)A–Ni(1)–O(1W)A	89.46(5)	O(1W)A–Ni(1)–N(1)	91.24(6)
O(2)–Ni(1)–O(1W)	89.46(6)	O(1W)–Ni(1)–N(1)	88.76(6)
O(2)A–Ni(1)–O(1W)	90.54(6)	O(2)–Ni(1)–N(1)A	89.58(6)
O(1W)A–Ni(1)–O(1W)	180.0	O(2)A–Ni(1)–N(1)A	90.42(6)
O(1W)A–Ni(1)–N(1)A	88.76(6)	N(1)–Ni(1)–N(1)A	180.0
O(1W)–Ni(1)–N(1)A	91.24(6)		

Symmetry codes: A: $-x + 1, -y, -z + 1$; B: $-x, -y - 1, -z$

Table S2 Selected bond distances (Å) and angles (deg) for complex **2**.

2			
Ni(1)–N(1)	2.108(2)	Ni(1)–N(1)A	2.108(2)
Ni(1)–O(2)	2.0187(15)	Ni(1)–O(2)A	2.0187(15)
Ni(1)–O(1W)	2.0899(16)	Ni(1)–O(1W)A	2.0899(16)
O(2)–Ni(1)–O(2)A	180.0	O(2)–Ni(1)–N(1)A	88.78(7)
O(2)–Ni(1)–O(1W)	87.85(7)	O(2)A–Ni(1)–N(1)A	91.23(7)
O(2)A–Ni(1)–O(1W)	92.14(7)	O(1W)–Ni(1)–N(1)A	91.13(8)
O(2)–Ni(1)–O(1W)A	92.15(7)	O(1W)A–Ni(1)–N(1)A	88.87(8)
O(2)A–Ni(1)–O(1W)A	87.86(7)	O(2)–Ni(1)–N(1)	91.22(7)
O(1W)–Ni(1)–O(1W)A	180.0	O(2)A–Ni(1)–N(1)	88.78(7)
O(1W)–Ni(1)–N(1)	88.87(8)	N(1)A–Ni(1)–N(1)	180.0
O(1W)A–Ni(1)–N(1)	91.13(8)		

Symmetry codes: A $-x, -y, -z$; B $-x + 1, -y, -z + 2$

Table S3 Selected bond distances (Å) and angles (deg) for complex **3**.

3			
Ni(1)–N(1)	2.1235(16)	Ni(1)–N(1)A	2.1235(16)
Ni(1)–O(3)	2.0673(13)	Ni(1)–O(3)A	2.0674(13)
Ni(1)–N(4)B	2.1448(16)	Ni(1)–N(4)C	2.1448(16)
O(3)–Ni(1)–O(3)A	180.0	N(1)–Ni(1)–N(4)B	84.98(6)
O(3)–Ni(1)–N(1)	86.53(6)	N(1)A–Ni(1)–N(4)B	95.02(6)
O(3)A–Ni(1)–N(1)	93.47(6)	O(3)–Ni(1)–N(4)C	86.28(6)
O(3)–Ni(1)–N(1)A	93.47(6)	O(3)A–Ni(1)–N(4)C	93.72(6)
O(3)A–Ni(1)–N(1)A	86.53(6)	N(1)–Ni(1)–N(4)C	95.02(6)
N(1)–Ni(1)–N(1)A	180.0	N(1)A–Ni(1)–N(4)C	84.98(6)
O(3)–Ni(1)–N(4)B	93.72(6)	N(4)B–Ni(1)–N(4)C	180.00(10)
O(3)A–Ni(1)–N(4)B	86.28(6)		

Symmetry codes: A $-x + 2, -y, -z$; B $x + 1, -y + 1/2, z - 1/2$; C $-x + 1, y - 1/2, -z + 1/2$

Table S4 Selected bond distances (Å) and angles (deg) for complex **4**.

4			
Ni(1)–N(1)	2.1330(18)	Ni(1)–N(1)A	2.1330(18)
Ni(1)–O(3)	2.0750(14)	Ni(1)–O(3)A	2.0750(14)
Ni(1)–N(4)B	2.1382(18)	Ni(1)–N(4)C	2.1382(18)
O(3)–Ni(1)–O(3)A	180.0	N(1)A–Ni(1)–N(4)B	93.46(7)
O(3)–Ni(1)–N(1)A	94.89(6)	N(1)–Ni(1)–N(4)B	86.54(7)
O(3)A–Ni(1)–N(1)A	85.11(6)	O(3)–Ni(1)–N(4)C	88.02(6)
O(3)–Ni(1)–N(1)	85.11(6)	O(3)A–Ni(1)–N(4)C	91.98(6)
O(3)A–Ni(1)–N(1)	94.89(6)	N(1)A–Ni(1)–N(4)C	86.54(7)
N(1)A–Ni(1)–N(1)	180.0	N(1)–Ni(1)–N(4)C	93.46(7)
O(3)–Ni(1)–N(4)B	91.98(6)	N(4)B–Ni(1)–N(4)C	180.0
O(3)A–Ni(1)–N(4)B	88.02(6)		

Symmetry codes: A $-x, -y, -z + 3$; B $x + 1, -y + 1/2, z + 3/2$; C $-x - 1, y - 1/2, -z + 3/2$

Table S5 Selected bond distances (Å) and angles (deg) for complex **5**.

5			
Ni(1)–N(1)	2.100(4)	Ni(1)–N(4)B	2.113(4)
Ni(1)–O(3)	2.062(3)	Ni(1)–O(5)	2.058(3)
Ni(1)–O(1W)	2.089(3)	Ni(1)–O(6)A	2.073(3)
O(5)–Ni(1)–O(3)	101.45(11)	O(6)A–Ni(1)–N(1)	90.73(13)
O(5)–Ni(1)–O(6)A	77.78(11)	O(1W)–Ni(1)–N(1)	91.75(13)
O(3)–Ni(1)–O(6)A	178.28(12)	O(5)–Ni(1)–N(4)B	91.35(13)
O(5)–Ni(1)–O(1W)	170.92(11)	O(3)–Ni(1)–N(4)B	90.74(12)
O(3)–Ni(1)–O(1W)	87.51(11)	O(6)A–Ni(1)–N(4)B	90.81(12)
O(6)A–Ni(1)–O(1W)	93.32(11)	O(1W)–Ni(1)–N(4)B	87.00(13)
O(5)–Ni(1)–N(1)	90.11(13)	N(1)–Ni(1)–N(4)B	178.07(14)
O(3)–Ni(1)–N(1)	87.73(13)		

Symmetry codes: A $-x + 1, y + 1/2, -z + 3/2$; B $x + 1, -y + 3/2, z + 1/2$

Table S6 Selected bond distances (Å) and angles (deg) for complex **6**.

6			
Ni(1)–N(1)	2.192(3)	Ni(1)–N(1)A	2.192(3)
Ni(1)–O(3)	2.018(3)	Ni(1)–O(3)A	2.018(3)
Ni(1)–O(1W)	2.059(3)	Ni(1)–O(1W)A	2.059(3)
Ni(2)–O(2W)	2.082(2)	Ni(2)–O(2W)B	2.082(2)
Ni(2)–O(5)	2.094(3)	Ni(2)–O(5)B	2.094(3)
Ni(2)–N(4)C	2.085(3)	Ni(2)–N(4)D	2.085(3)
O(3)–Ni(1)–O(3)A	180.0	O(3)–Ni(1)–N(1)	87.93(12)
O(3)–Ni(1)–O(1W)A	90.93(11)	O(3)A–Ni(1)–N(1)	92.07(12)
O(3)A–Ni(1)–O(1W)A	89.07(11)	O(1W)A–Ni(1)–N(1)	91.00(12)
O(3)–Ni(1)–O(1W)	89.07(11)	O(1W)–Ni(1)–N(1)	89.00(12)
O(3)A–Ni(1)–O(1W)	90.93(11)	N(1)A–Ni(1)–N(1)	180.00(17)
O(1W)A–Ni(1)–O(1W)	180.0	O(2W)–Ni(2)–O(2W)B	180.0
O(3)–Ni(1)–N(1)A	92.07(12)	O(2W)–Ni(2)–N(4)C	85.67(12)
O(3)A–Ni(1)–N(1)A	87.93(12)	O(2W)B–Ni(2)–N(4)C	94.33(12)
O(1W)A–Ni(1)–N(1)A	89.00(12)	O(2W)–Ni(2)–N(4)D	94.33(12)
O(1W)–Ni(1)–N(1)A	91.00(12)	O(2W)B–Ni(2)–N(4)D	85.67(12)
N(4)C–Ni(2)–N(4)D	180.0	O(2W)B–Ni(2)–O(5)B	88.29(10)
O(2W)–Ni(2)–O(5)	88.29(10)	N(4)C–Ni(2)–O(5)B	91.38(12)
O(2W)B–Ni(2)–O(5)	91.71(10)	N(4)D–Ni(2)–O(5)B	88.62(12)
N(4)C–Ni(2)–O(5)	88.62(12)	O(5)–Ni(2)–O(5)B	180.0
N(4)D–Ni(2)–O(5)	91.38(12)	O(2W)–Ni(2)–O(5)B	91.71(10)

Symmetry codes: A $-x + 1, -y + 1, -z + 1$; B $-x, -y, -z + 2$; C $-x + 1, -y + 2, -z + 2$; D $x - 1, y - 2, z$

Table S7 Selected bond distances (Å) and angles (deg) for complex **7**.

7			
Ni(1)–N(1)	2.139(6)	Ni(1)–N(4)B	2.112(6)
Ni(1)–O(3)	2.090(4)	Ni(1)–O(6)A	2.054(4)
Ni(1)–O(1W)	2.072(4)	Ni(1)–O(2W)	2.051(5)
O(6)A–Ni(1)–O(2W)	91.87(18)	O(6)A–Ni(1)–N(4)B	88.4(2)
O(6)A–Ni(1)–O(1W)	88.57(18)	O(2W)–Ni(1)–N(4)B	87.8(2)
O(2W)–Ni(1)–O(1W)	179.0(2)	O(1W)–Ni(1)–N(4)B	91.3(2)
O(6)A–Ni(1)–O(3)	178.3(2)	O(3)–Ni(1)–N(4)B	93.2(2)
O(2W)–Ni(1)–O(3)	87.61(19)	O(6)A–Ni(1)–N(1)	89.3(2)
O(1W)–Ni(1)–O(3)	91.97(19)	O(2W)–Ni(1)–N(1)	92.1(2)
O(3)–Ni(1)–N(1)	89.1(2)	O(1W)–Ni(1)–N(1)	88.8(2)
N(4)B–Ni(1)–N(1)	177.6(3)		

Symmetry codes: A x, $-y + 2$, $z - 1/2$; B $x - 1/2$, $y + 1/2$, $z + 1$

Table S8 Selected bond distances (Å) and angles (deg) for complex **8**.

8			
Ni(1)–N(2)	2.041(3)	Ni(1)–O(1)	2.047(3)
Ni(1)–N(1)	2.055(3)	Ni(1)–O(4)A	2.067(3)
Ni(1)–O(3)A	2.146(3)	Ni(1)–O(2)	2.186(3)
N(2)–Ni(1)–O(1)	96.85(12)	N(2)–Ni(1)–N(1)	97.95(12)
O(1)–Ni(1)–N(1)	94.63(12)	N(2)–Ni(1)–O(4)A	99.62(12)
O(1)–Ni(1)–O(4)A	155.36(11)	N(1)–Ni(1)–O(4)A	101.06(12)
N(2)–Ni(1)–O(3)A	88.67(11)	O(1)–Ni(1)–O(3)A	99.82(11)
N(1)–Ni(1)–O(3)A	163.29(12)	O(4)A–Ni(1)–O(3)A	62.57(10)
N(2)–Ni(1)–O(2)	157.46(12)	O(1)–Ni(1)–O(2)	62.26(10)
N(1)–Ni(1)–O(2)	92.47(12)	O(4)A–Ni(1)–O(2)	97.90(11)
O(3)A–Ni(1)–O(2)	86.91(10)		

Symmetry code: A: x, $y + 1$, z

Table S9 Selected bond distances (Å) and angles (deg) for complex **9**.

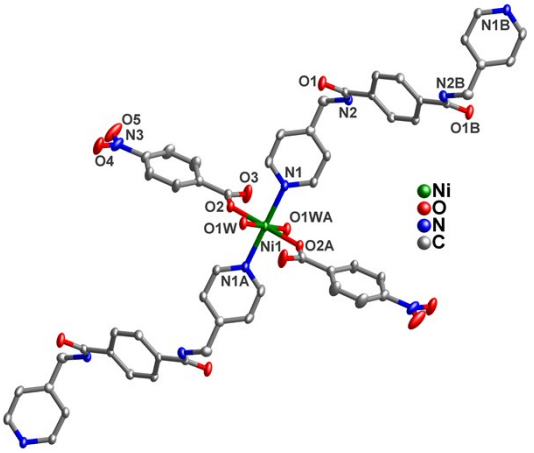
9			
Ni(1)–N(1)	2.114(4)	Ni(1)–N(1)A	2.114(4)
Ni(1)–O(2)	2.028(3)	Ni(1)–O(2)A	2.028(3)
Ni(1)–O(1)	2.073(3)	Ni(1)–O(1)A	2.073(3)
O(2)A–Ni(1)–O(2)	180.0	O(2)A–Ni(1)–O(1)	88.59(12)
O(2)–Ni(1)–O(1)	91.41(12)	O(2)A–Ni(1)–O(1)A	91.41(12)
O(2)–Ni(1)–O(1)A	88.59(12)	O(1)–Ni(1)–O(1)A	180.0
O(1)–Ni(1)–N(1)	89.07(14)	O(1)A–Ni(1)–N(1)	90.93(14)
O(2)A–Ni(1)–N(1)A	89.49(13)	O(2)–Ni(1)–N(1)A	90.51(13)
O(1)–Ni(1)–N(1)A	90.93(14)	O(1)A–Ni(1)–N(1)A	89.07(14)
O(2)A–Ni(1)–N(1)	90.51(13)	O(2)–Ni(1)–N(1)	89.49(13)
N(1)A–Ni(1)–N(1)	180.0		

Symmetry code: A: –*x*, –*y*, –*z*

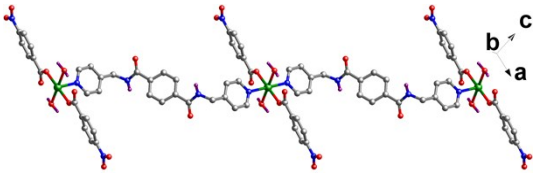
Table S10 Selected bond distances (Å) and angles (deg) for complex **10**.

10			
Ni(1)–O(1W)A	2.0657(13)	Ni(1)–O(1W)	2.0657(13)
Ni(1)–O(1)A	2.1020(11)	Ni(1)–O(1)	2.1020(11)
Ni(1)–N(1)	2.1065(14)	Ni(1)–N(1)A	2.1065(14)
O(1W)A–Ni(1)–O(1W)	180.0	O(1W)A–Ni(1)–O(1)A	88.26(5)
O(1W)–Ni(1)–O(1)A	91.74(5)	O(1W)A–Ni(1)–O(1)	91.74(5)
O(1W)–Ni(1)–O(1)	88.26(5)	O(1)A–Ni(1)–O(1)	180.0
O(1W)A–Ni(1)–N(1)	87.85(6)	O(1W)–Ni(1)–N(1)	92.14(6)
O(1)A–Ni(1)–N(1)	91.18(5)	O(1)–Ni(1)–N(1)	88.82(5)
O(1W)A–Ni(1)–N(1)A	92.15(6)	O(1W)–Ni(1)–N(1)A	87.85(6)
O(1)A–Ni(1)–N(1)A	88.82(5)	O(1)–Ni(1)–N(1)A	91.18(5)
N(1)–Ni(1)–N(1)A	180.0		

Symmetry code: A: –*x*, –*y*, –*z*

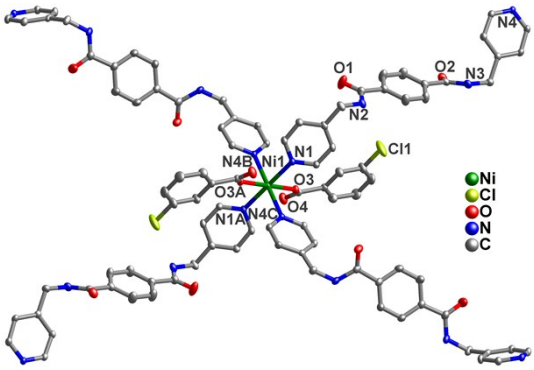


(a)

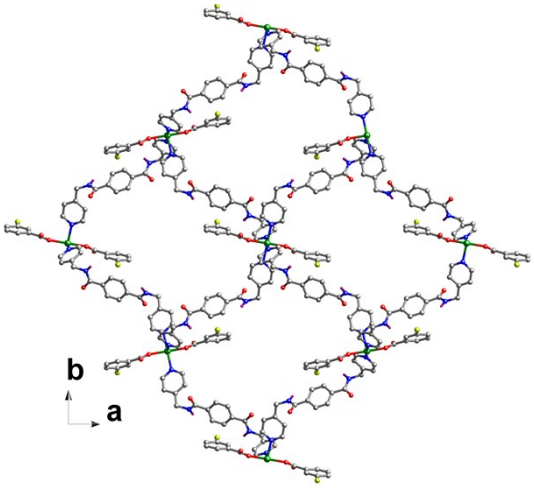


(b)

Fig. S1 (a) The coordination environment of Ni(II) ion in **2**; (b) 1D chain extended by L.

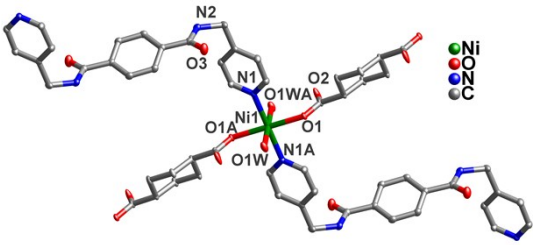


(a)

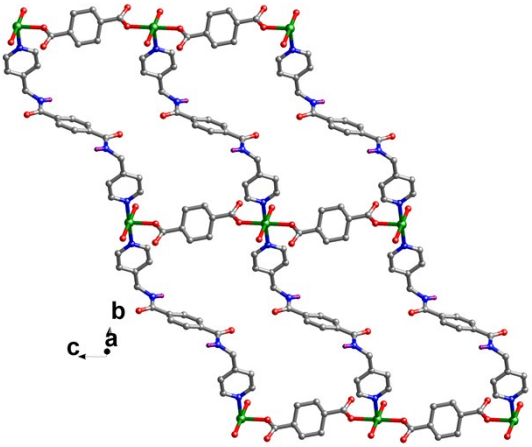


(b)

Fig. S2 (a) The coordination environment of Ni(II) ion in **4**; (b) The 2D network.



(a)



(b)

Fig. S3 (a) The coordination environment of Ni(II) ion in **10**; (b) The 2D network.

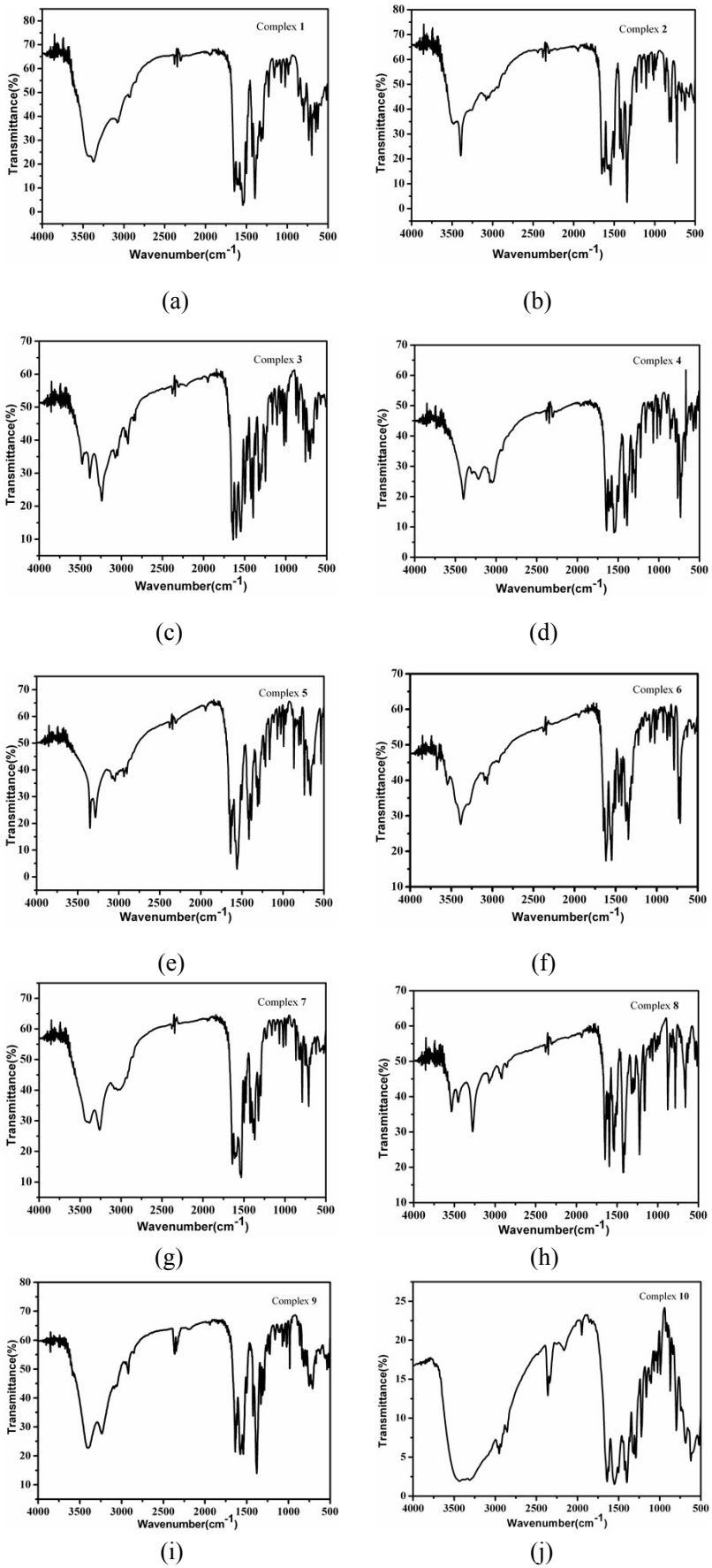


Fig. S4 The IR spectra of complexes **1–10**.

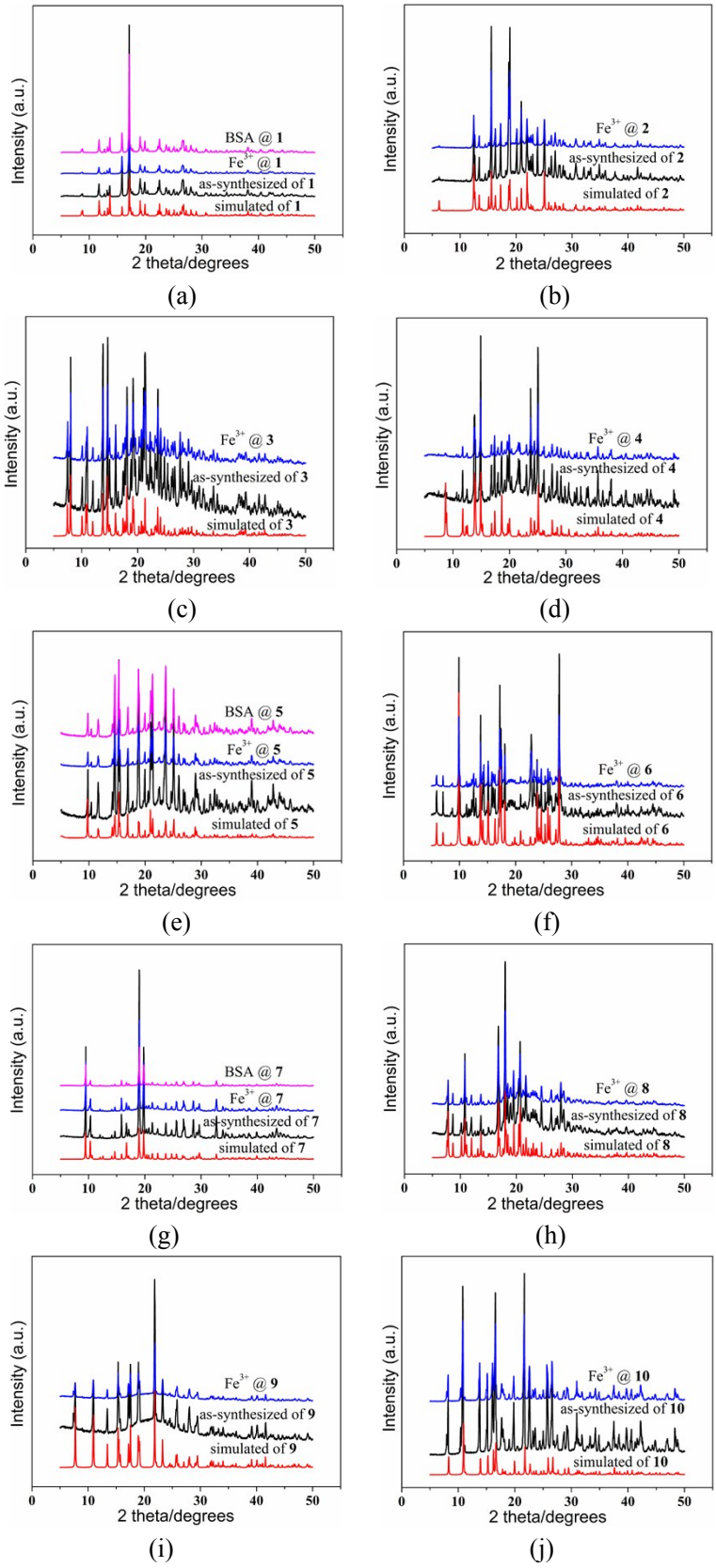


Fig. S5 The PXRD patterns of complexes **1**–**10**.

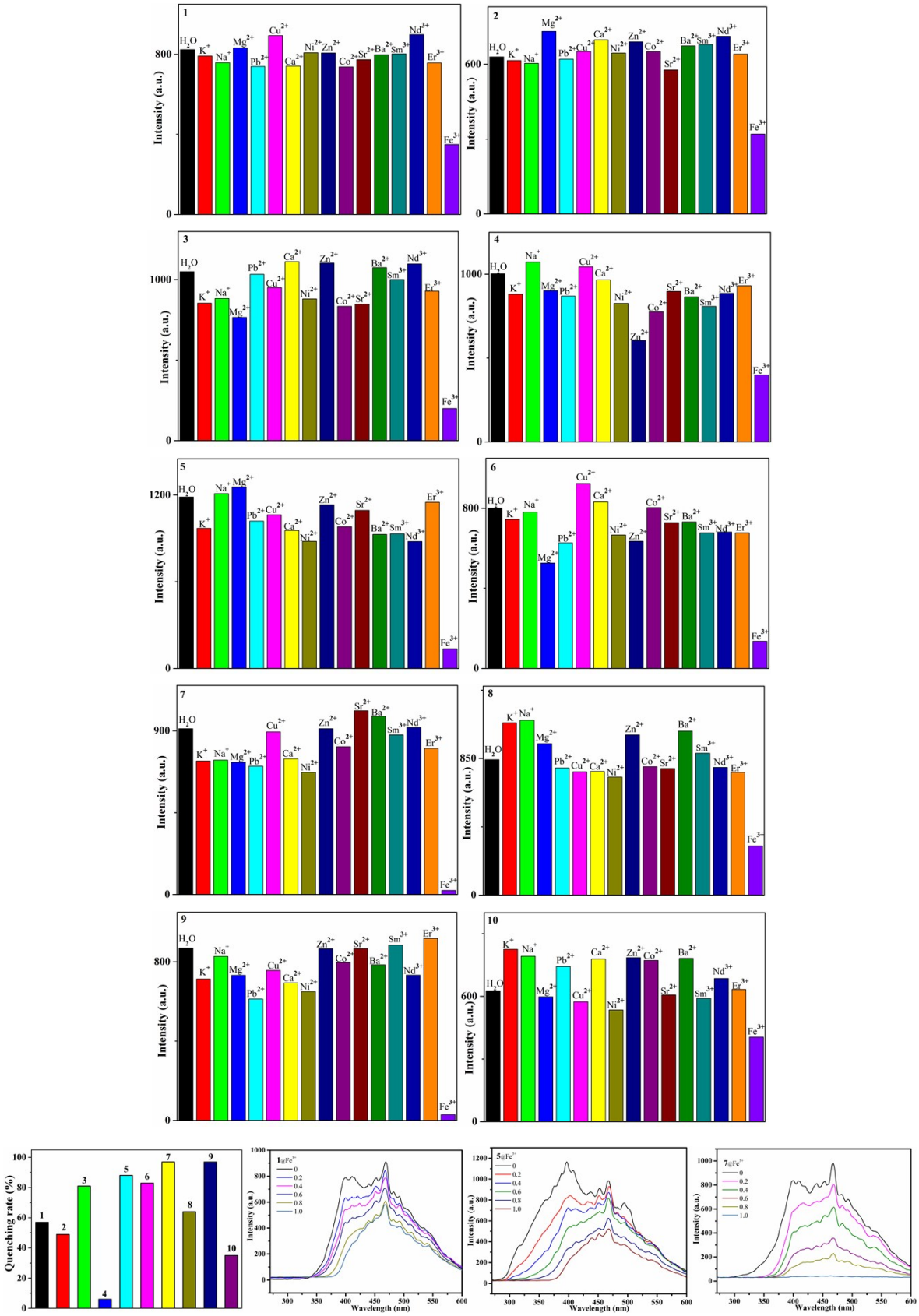
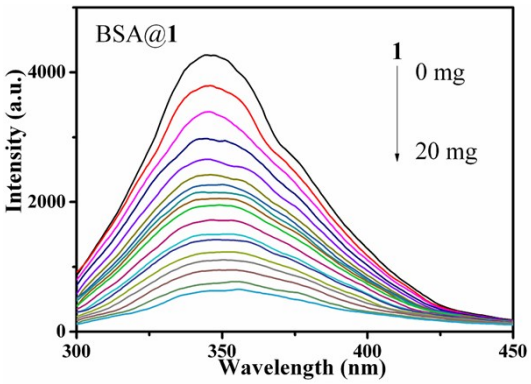
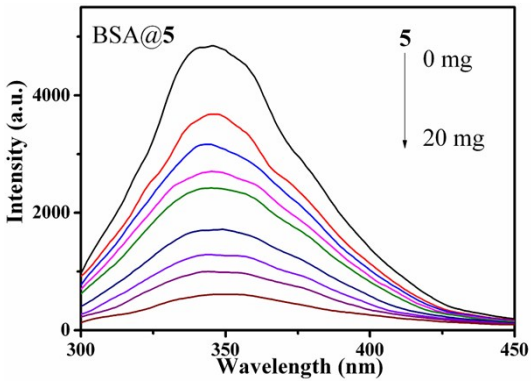


Fig. S6 Luminescence spectra of M^{n+}@**1–10**, the Luminescent quenching rates of **1–10** induced by Fe^{3+} and the emission spectra of Fe^{3+}@**1**, **5**, **7** aqueous suspensions with the concentration of Fe^{3+}.

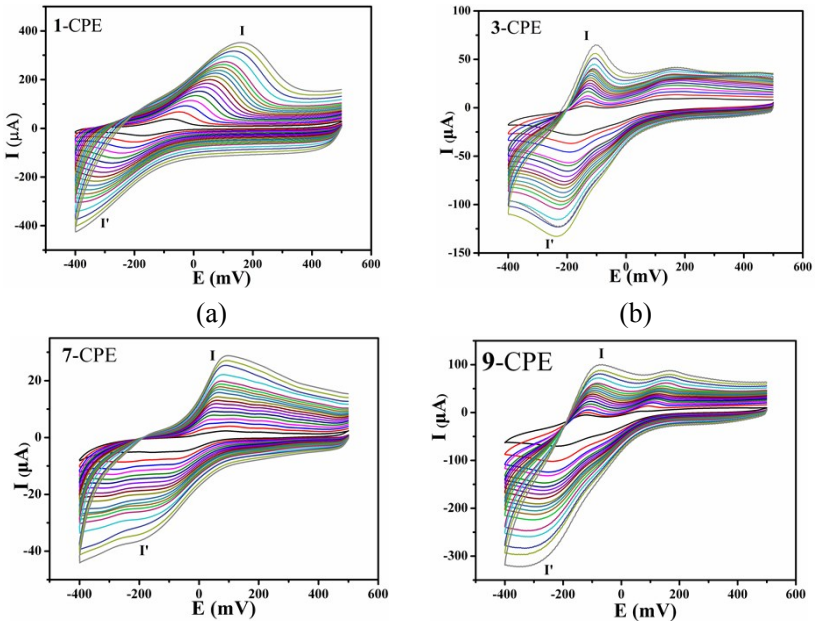


(a)



(b)

Fig. S7 Fluorescence spectra of BSA with different concentrations of complex **1** (a) and **5** (b).



(a) (b) (c) (d)

Fig. S8 Cyclic voltammograms of **1**-, **3**-, **7**-, **9**-CPE in 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution at different scan rates. Scan rates from 20 to 400 mVs^{-1}.

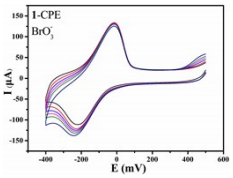
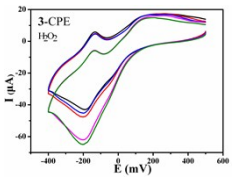
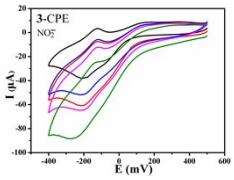
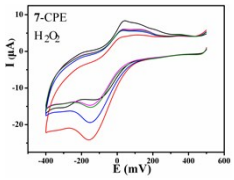
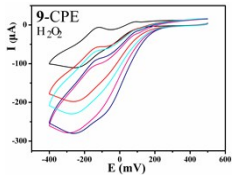
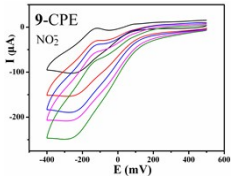
Complexes	H_2O_2	BrO_3^-	NO_2^-
1			
3			
5			
7			
9			

Fig. S9 The different electrochemical activities.

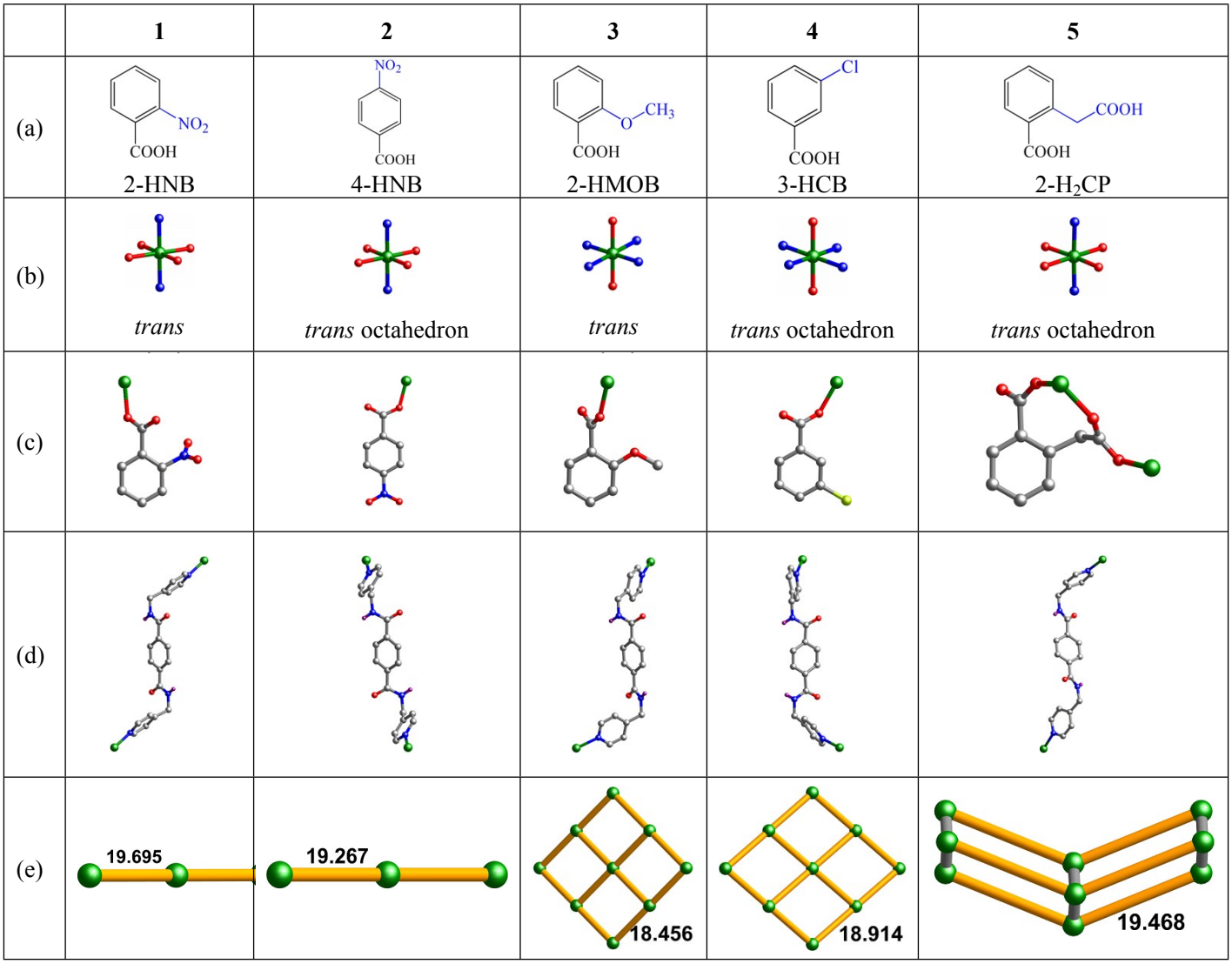


Chart S1 The structural details of complexes **1**–**5**. (a) The carboxylic acids; (b) The coordination modes of Ni(II); (c) The subunits of Ni-carboxylates; (d) The subunits of Ni-L; (e) The schematic view of the structures.

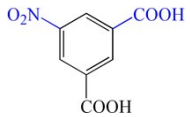
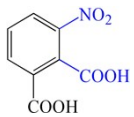
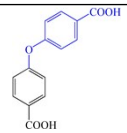
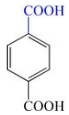
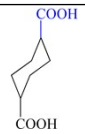
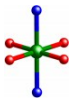
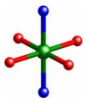
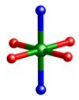
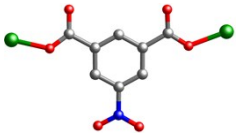
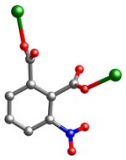
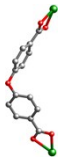
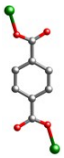
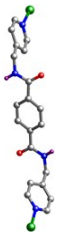
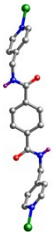
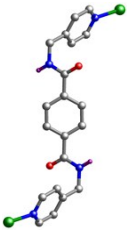
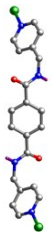
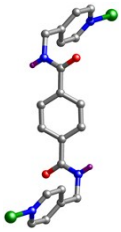
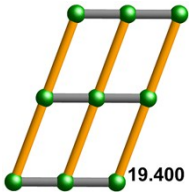
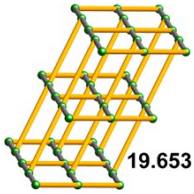
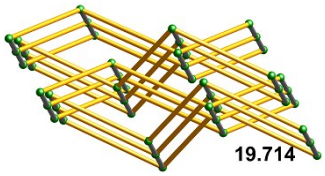
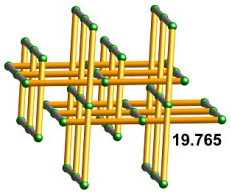
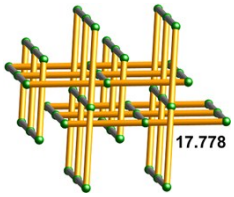
	6	**7**	**8**	**9**	**10**
(a)	 5-H_2NIP	 3-H_2NP	 4,4′-H_2OBA	 1,4-H_2BDC	 1,4-H_2CHDA
(b)	 *trans* octahedron	 *trans*	 *cis* octahedron	 *trans* octahedron	 *trans* octahedron
(c)					
(d)					
(e)					

Chart S2 The structural details of complexes **6**–**10**. (a) The carboxylic acids; (b) The coordination modes of Ni(II); (c) The subunits of Ni-carboxylates; (d) The subunits of Ni-L; (e) The schematic view of the structures.

Complexes	H_2O_2	BrO_3^-	NO_2^-
1			
3			
5			
7			
9			

Chart S3 The different electrochemical activities.