Electronic Supplementary Information (ESI)

Syntheses, structures and chemical sensing properties of three complexes with mixed ligands of carboxylate and bipyridine

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Table S1. Crystal data and structure refinements for complexes **1** and **3**.

	1	**3**
chemical formula	$C_{28}H_{24}Cu_2N_4O_{10}$	$C_{18}H_{28}N_2Ni_2O_{16}$
formula Mass	703.59	645.80
crystal system	Monoclinic	Monoclinic
Space group	*P2(1)/c*	*P21/c*
a (Å)	9.731(5)	6.162(4)
b (Å)	13.576(7)	20.190(11)
c (Å)	10.412(6)	10.193(6)
α (deg)	90.00	90.00
β (deg)	94.825(7)	105.181(6)
γ (deg)	90.00	90.00
V (Å^3)	1370.7(13)	1223.9(13)
Z	2	2
T (K)	293(2)	293(2)
No. of reflections measured	6370	6542
No. of independent reflections	2398	2697
R_{int}	0.0309	0.0362
Final R_1 values $[I > 2\sigma(I)]^a$	0.0313	0.0385
wR_2 $[I > 2\sigma(I)]$	0.0713	0.0896
Final R_1 values (all data)	0.0504	0.0601
wR_2 (all data)^b	0.0800	0.1008
Goodness of fit on F^2	1.021	0.975

^{a} $R_1 = \Sigma\ (|F_0|-|F_C|) / \Sigma\ |F_0|$; ^{b} $wR_2 = [\Sigma\ w\ (|F_0|-|F_C|)^2 / \Sigma\ w\ F_0^2]^{1/2}$

Table S2. The selected bond lengths [Å] and angles [°] of complex **1**.

Cu(1)-O(4)	1.926(2)	Cu(1)-N(2)	2.013(3)
Cu(1)-O(1)	2.000(2)	Cu(1)-O(1)#1	2.346(2)
Cu(1)-N(1)	2.007(2)	Cu(1)-O(3)	2.411(2)
O(4)-Cu(1)-O(1)	91.41(10)	N(1)-Cu(1)-O(1)#1	96.39(9)
O(4)-Cu(1)-N(1)	171.59(9)	N(2)-Cu(1)-O(1)#1	112.22(9)
O(1)-Cu(1)-N(1)	94.58(10)	O(4)-Cu(1)-O(3)	78.63(9)
O(4)-Cu(1)-N(2)	92.86(10)	O(1)-Cu(1)-O(3)	75.75(8)
O(1)-Cu(1)-N(2)	171.29(9)	N(1)-Cu(1)-O(3)	97.11(10)
N(1)-Cu(1)-N(2)	80.44(10)	N(2)-Cu(1)-O(3)	97.66(9)
O(4)-Cu(1)-O(1)#1	90.84(9)	O(1)#1-Cu(1)-O(3)	148.84(7)
O(1)-Cu(1)-O(1)#1	75.28(9)	C(12)-O(3)-C(13)	114.5(3)

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

Table S3. The selected bond lengths [Å] and angles [º] of complex **3**.

Ni(1)-O(3)	2.033(2)	Ni(1)-O(7)	2.050(2)
Ni(1)-N(1)	2.038(3)	Ni(1)-O(6)	2.054(2)
Ni(1)-O(5)	2.050(2)	Ni(1)-O(13)	2.074(2)
O(3)-Ni(1)-N(1)	177.26(9)	O(3)-Ni(1)-O(13)	89.72(9)
O(3)-Ni(1)-O(5)	79.25(8)	N(1)-Ni(1)-O(13)	92.99(9)
N(1)-Ni(1)-O(5)	101.26(9)	O(5)-Ni(1)-O(13)	87.86(10)
O(3)-Ni(1)-O(7)	79.00(8)	O(7)-Ni(1)-O(13)	90.22(10)
N(1)-Ni(1)-O(7)	100.55(9)	O(6)-Ni(1)-O(13)	174.95(9)
O(5)-Ni(1)-O(7)	158.17(8)	C(7)-O(3)-C(8)	119.8(2)
O(3)-Ni(1)-O(6)	87.72(8)	C(7)-O(3)-Ni(1)	114.64(16)
N(1)-Ni(1)-O(6)	89.61(8)	C(8)-O(3)-Ni(1)	114.34(17)
O(5)-Ni(1)-O(6)	87.38(10)	C(6)-O(7)-Ni(1)	115.94(18)
O(7)-Ni(1)-O(6)	93.57(10)	C(9)-O(5)-Ni(1)	116.09(18)
O(3)-Ni(1)-N(1)	177.26(9)	O(3)-Ni(1)-O(13)	89.72(9)

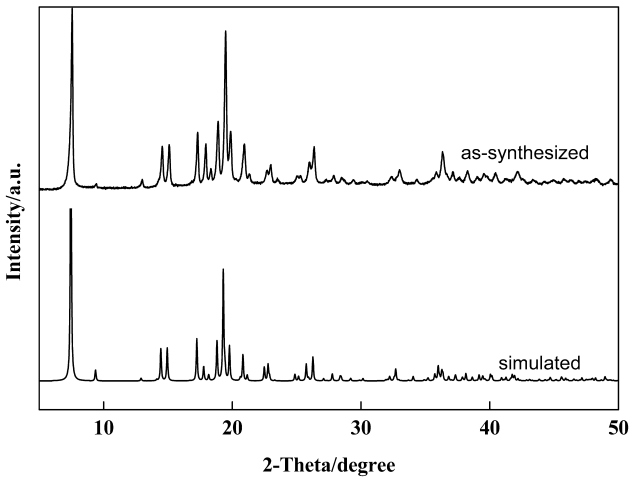

Fig. S1. Experimental powder X-Ray diffraction pattern of as-synthesized $Ni_2(oda)_2(4,4'\text{-bipy})\cdot DMF$ (complex **2**) and the simulated one based on the crystal structure of $Co_2(oda)_2(4,4'\text{-bipy})\cdot DMF$ we have reported recently.

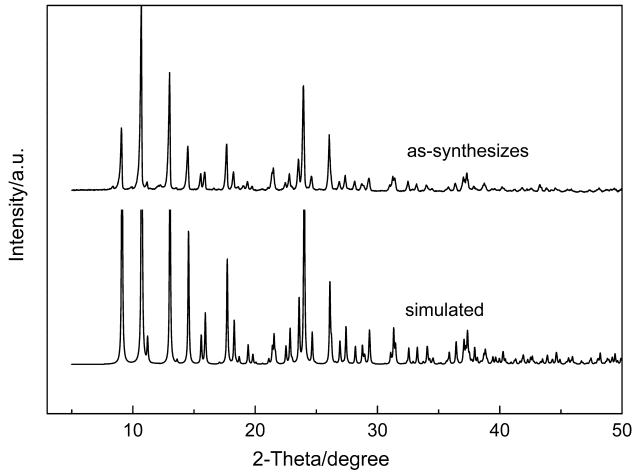

Fig. S2. Simulated and measured PXRD patterns for complex **1**.

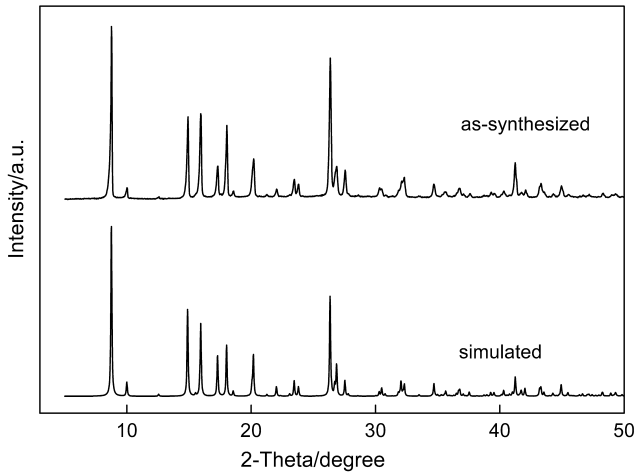

Fig. S3. Simulated and measured PXRD patterns for complex **3**.

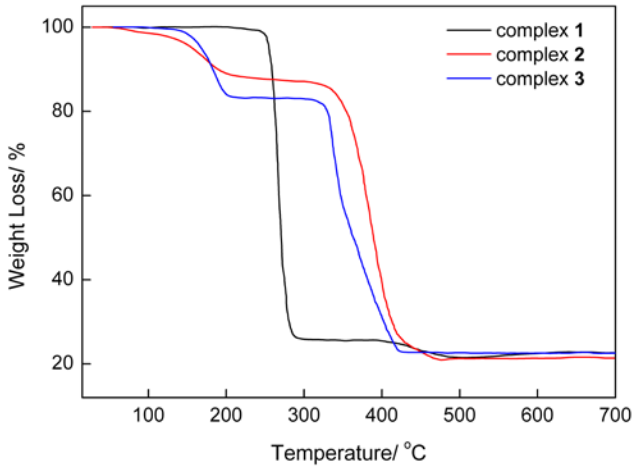

Fig. S4. Thermogravimetric analysis (TGA) curves of complexes **1**, **2** and **3**.

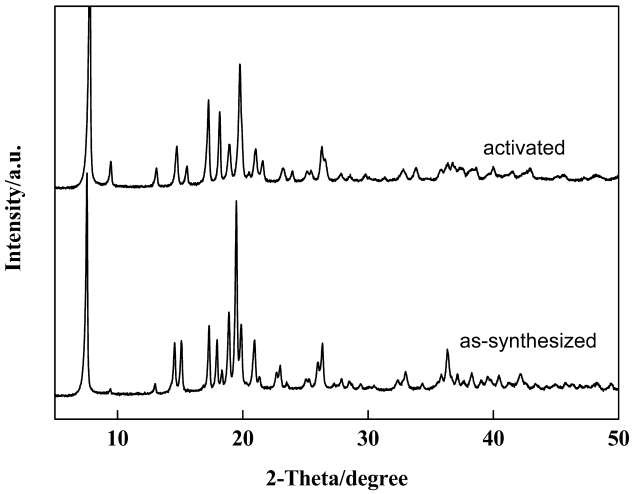

Fig. S5. PXRD patterns of the as-synthesized and the activated complex **2**.

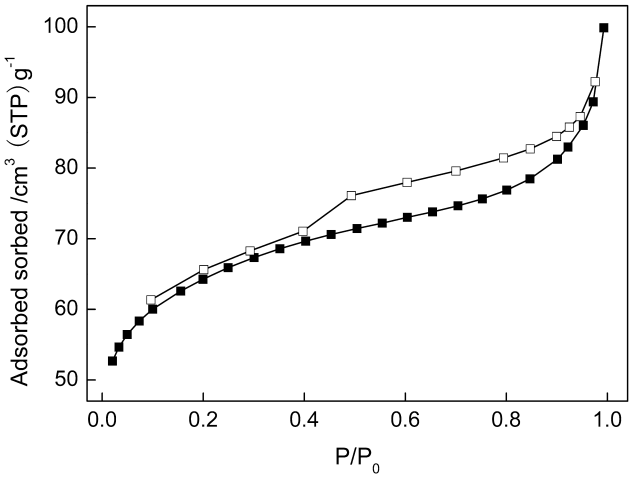

Fig. S6. N_2 sorption isotherms of complex **2** at 77 K. Closed and open symbols represent adsorption and desorption, respectively.

Authors' Contributions

Chengli Jiao managed the crystal syntheses, structures analyses, QCM tests and manuscript preparation. Fen Li managed the structure refinement of complex **2**. Jian Zhang and Shuang Wang managed the thermogravimetric analyses. Zhangpeng Li managed the crystal structures analyses and refinements. Zhonggang Wang and Hao Yu managed the crystal structures data collection. Zhibao Li, Shuang Liu, Ziqiang Wang and Xia Jiang managed the powder X-ray diffraction patterns collection. Lixian Sun and Fen Xu established the direction of this project including funding of the research, designed the experiment and revised the manuscript.