Supporting Information

Crystal structure and oxygen reduction reaction of Ni(II) complex template Borate-sulfate and Borate

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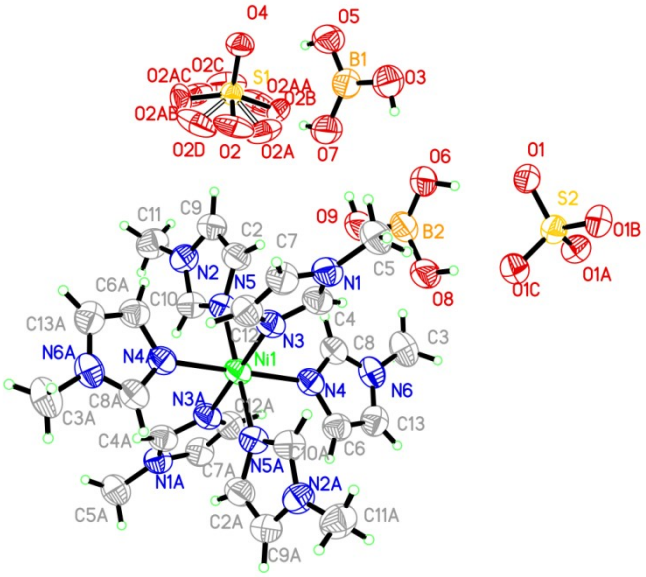

Fig. S1 ORTEP view of **1** made at the 30% probability level.

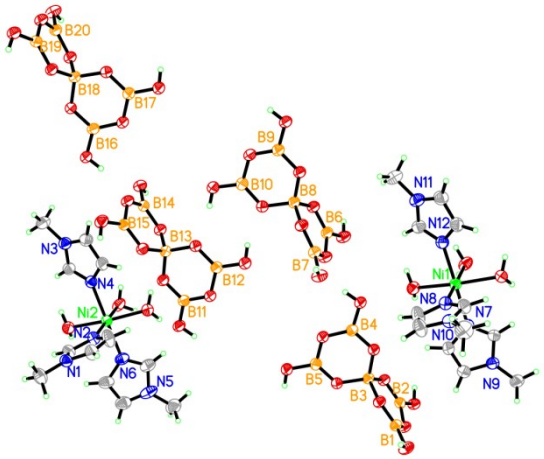

Fig. S2 ORTEP view of **2** made at the 30% probability level; C (gray), O (red), and H (white).

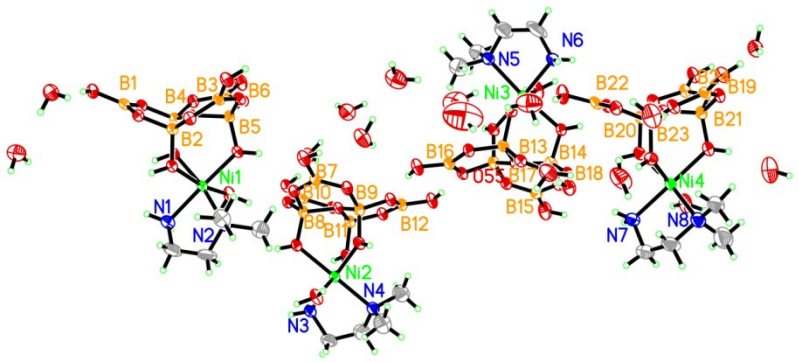

Fig. S3 ORTEP view of **3** made at the 30% probability level; C (gray), O (red), and H (white).

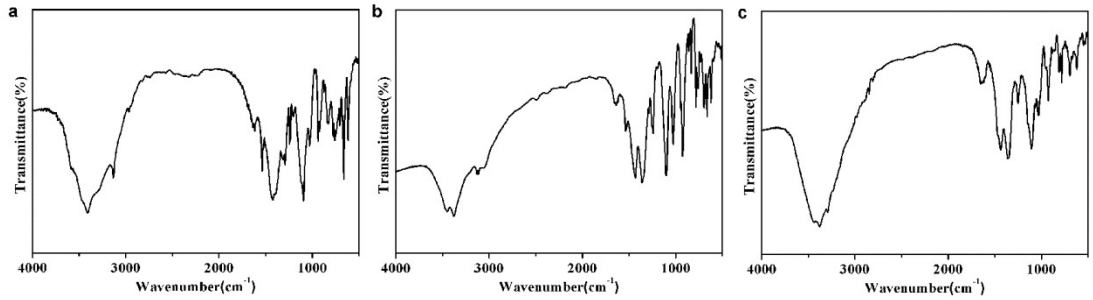

Fig. S4 The FTIR spectra of compound **1**–**3**.

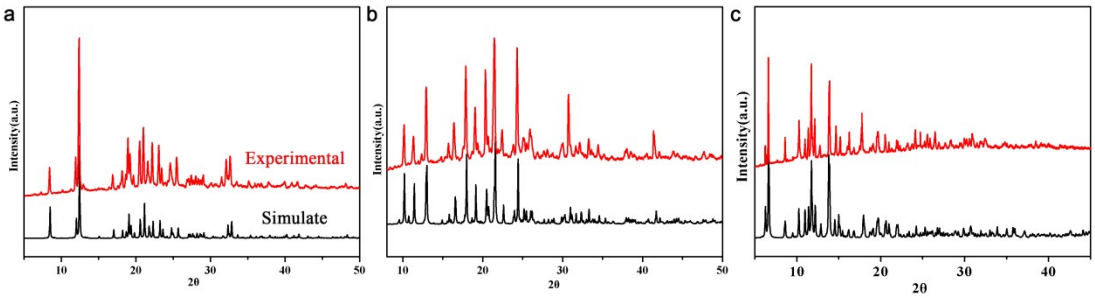

Fig. S5 The PXRD patterns of compound **1** (a), **2** (b) and **3** (c).

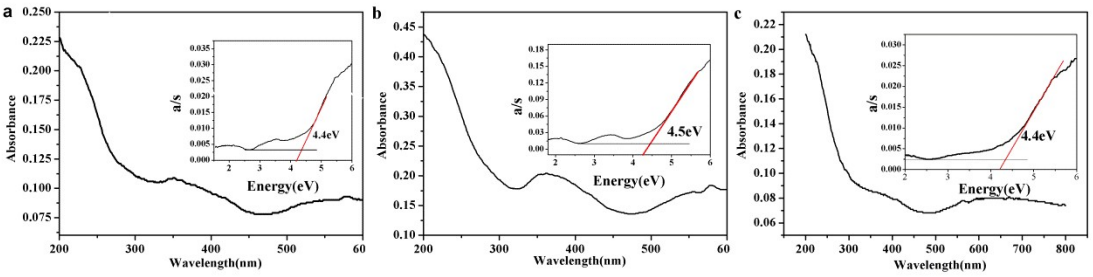

Fig. S6 The solid-state UV-vis absorption spectra of compound **1**(a), **2**(b) and **3** (c) (the insets show the Tauc plots of *α/S* vs. photon energy).

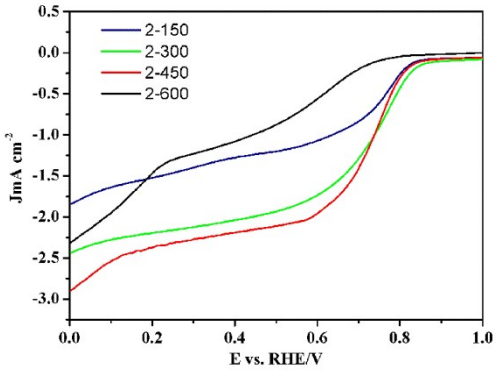

Fig. S7 LSV curves of 2-150, 2-300, 2-450 and 2-600 (5 mV/s, 1600 rpm). The LSV curve of 2-450 presented an $E_{1/2}$ at the potential of 0.74 V.

Table S1 Details of hydrogen bond for **1**.

D–H···A	d(D–H)(Å)	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O4—H4···O3	0.84	1.87	2.684(2)	164.4
O5—H5A···O3[1]	0.84	1.92	2.749(2)	171.6
O6—H6A···O7	0.84	1.91	2.749(3)	174.4
O7—H7A···O1	0.84	2.02	2.79(2)	153.4
O7—H7A···O1A	0.84	1.69	2.509(7)	165.6
O8—H8···O4	0.84	1.97	2.782(3)	162.8
O9—H9A···O2	0.84	2.06	2.880(2)	163.3

[1]1-Y, -1/2+X, 1-Z

Table S2 Details of hydrogen bond for **2**.

D–H···A	d(D–H)(Å)	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1—H1···O14[5]	0.84	1.91	2.739(2)	169.3
O3—H3A···O15[6]	0.84	1.87	2.708(2)	173.2
O8—H8A···O34[7]	0.84	1.88	2.717(2)	171.6
O10—H 10A···O12	0.84	1.92	2.695(2)	152.8
O11—H11A···O5[5]	0.84	1.96	2.784(2)	167.4
O13—H13···O4[6]	0.84	2.05	2.874(2)	167.9
O18—H18A···O24	0.84	1.95	2.785(2)	171.5
O20—H20···O2[8]	0.84	1.92	2.736(2)	164.4
O21—H21A···O39[7]	0.84	1.95	2.710(2)	150.9

O23—H23A···O17	0.84	1.88	2.697(2)	164.7
O28—H28···O27[9]	0.84	1.98	2.807(2)	169.6
O30—H30···O26[10]	0.84	1.99	2.810(2)	165.4
O31—H31···O29	0.84	1.89	2.706(2)	164.0
O33—H33···O6[8]	0.84	1.93	2.766(2)	173.4
O38—H38···O37[11]	0.84	1.91	2.750(2)	173.0
O40—H40···O36[12]	0.84	1.92	2.753(2)	175.3
O42—H42A···O40[4]	0.88	1.99	2.851(2)	165.8
O45—H45A···O1[2]	0.88	2.02	2.853(2)	159.4

[1]1/2+X,3/2-Y,1/2+Z; [2]2-X,1-Y,1-Z; [3]1/2+X,3/2-Y,-1/2+Z; [4]1/2-X,-1/2+Y,1/2-Z; [5]3/2-X,-1/2+Y,1/2-Z; [6]3/2-X,1/2+Y,1/2-Z; [7]1+X,+Y,+Z; [8]-1+X,+Y,+Z; [9]1-X,1-Y,1-Z; [10]1-X,2-Y,1-Z; [11]-X,1-Y,1-Z; [12]-X,2-Y,1-Z

Table S3 Details of hydrogen bond for **3**.

D–H···A	d(D–H)(Å)	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1—H1···O66	0.84	1.91	2.728	165.9
O5—H5···O48[1]	0.84	1.93	2.770	175.2
O8—H8···O15[2]	0.88	2.18	2.876	136.5
O11—H11···O24	0.88	1.90	2.769	175.1
O12—H12···O19[2]	0.84	1.93	2.756	167.4
O13—H13···O9[3]	0.84	1.88	2.723	177.0
O14—H14A···O12[2]	0.87	2.14	2.775	129.2
O14—H14B···O22	0.88	2.01	2.709	136.0
O15—H15···O68	0.84	1.84	2.632	155.7
O18—H18···O33	0.84	1.93	2.765	177.5
O24—H24···O65	0.84	1.96	2.763	160.3
O26—H26···O58[4]	0.84	1.94	2.750	162.9
O27—H27···O1[2]	0.84	2.02	2.851	168.3
O42—H42···O60	0.84	1.98	2.802	165.4
O45—H45···O6[1]	0.84	1.91	2.747	175.8
O51—H51···O56	0.81	2.01	2.802	167.5
O53—H53···O57	0.87	1.95	2.797	164.3
O54—H54···O59	0.87	2.02	2.870	164.3
O55—H55B···O18[5]	0.87	2.09	2.840	144.5

O29—H29···O21	0.84	1.84	2.671	172.1
O32—H32···O61	0.84	1.90	2.717	165.7
O38—H38···O37[5]	0.84	1.92	2.718	158.2
O39—H39···O51[6]	0.84	1.94	2.767	170.3
O40—H40···O46	0.88	2.04	2.847	151.8
O41—H41A···O40[6]	0.87	1.98	2.760	149.1
O41—H41B···O49[6]	0.87	2.01	2.843	161.2
O70—H70···O42	0.88	1.95	2.746	148.4
O62—H62A···O63	0.87	2.02	2.620	125.6
O65—H65A···O64	0.87	1.90	2.770	175.9
O67—H67A···O4[7]	0.87	2.01	2.876	171.1
O67—H67B···O16[2]	0.87	1.94	2.786	162.4
O69—H69B···O66[3]	0.87	2.15	2.853	137.9
O61—H61A···O31[4]	0.87	2.02	2.873	166.2
O61—H61B···O59	0.87	1.92	2.779	169.1
O64—H64A···O63	0.87	1.95	2.666	139.3
O64—H64B···O43[1]	0.87	1.99	2.846	169.5
O66—H66A···O68[8]	0.87	1.97	2.812	161.1
O66—H66B···O67	0.87	1.90	2.759	170.1
O58—H58A···O64[1]	0.87	2.09	2.810	140.2
O58—H58B···O44	0.87	1.91	2.741	160.1
O68—H68A···O2[9]	0.90	1.90	2.770	163.0
O68—H68B···O69	0.87	1.87	2.733	173.5
O59—H59A···O58	0.87	2.14	2.826	135.7
O60—H60A···O62	0.87	2.00	2.680	133.8
O60—H60B···O61	0.87	1.99	2.815	156.9
O63—H63A···O60[1]	0.87	2.26	2.813	121.0
O63—H63B···O30	0.87	1.96	2.806	163.2

[1]-X, 1-Y, 1-Z; [2]1-X, 1-Y, -Z; [3]-X, 1-Y, -Z; [4]1-X, 1-Y, 1-Z; [5]1-X, 2-Y, 1-Z; [6]-X, 2-Y, 1-Z; [7]1-X, -Y, -Z; [8]+X, -1+Y, +Z; [9]+X, 1+Y, +Z