Ligand Substitution Induced Single-Crystal-to-Single-Crystal Transformations in Two Ni(II) Coordination Compounds Displaying Consequential Changes in Proton Conductivity

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STable. 1. Selected bond lengths (Å) and band angles (°) for compounds **1**.

Ni(1)-N(3)	2.048(3)	Ni(1)-N(4)	2.049(3)
Ni(1)-N(2)	2.057(3)	Ni(1)-O(1)	2.058(3)
Ni(1)-N(1)	2.060(3)	Ni(1)-O(2)	2.205(3)
N(3)-Ni(1)-N(4)	79.66(13)	N(3)-Ni(1)-N(2)	95.28(12)
N(4)-Ni(1)-N(2)	93.62(12)	N(3)-Ni(1)-O(1)	90.89(12)
N(4)-Ni(1)-O(1)	95.45(11)	N(2)-Ni(1)-O(1)	169.82(12)
N(3)-Ni(1)-N(1)	172.78(12)	N(4)-Ni(1)-N(1)	104.29(13)
N(2)-Ni(1)-N(1)	78.54(12)	O(1)-Ni(1)-N(1)	94.71(12)
N(3)-Ni(1)-O(2)	90.76(12)	N(4)-Ni(1)-O(2)	155.29(11)
N(2)-Ni(1)-O(2)	110.02(11)	O(1)-Ni(1)-O(2)	61.70(10)
N(1)-Ni(1)-O(2)	87.88(12)		

STable. 2. Selected bond lengths (Å) and band angles (°) for compound **2**

Ni(1)-O(4)	2.035(3)	Ni(1)-O(8)	2.059(3)
Ni(1)-O(9)	2.061(3)	Ni(1)-N(1)	2.073(3)
Ni(1)-O(7)	2.074(3)	Ni(1)-N(2)	2.083(3)
Ni(2)-O(18)	2.023(3)	Ni(2)-N(4)	2.063(3)
Ni(2)-O(20)	2.064(3)	Ni(2)-N(3)	2.072(3)
Ni(2)-O(17)	2.108(3)	Ni(2)-O(16)	2.202(2)
O(4)-Ni(1)-O(8)	89.56(11)	O(4)-Ni(1)-O(9)	92.14(12)
O(8)-Ni(1)-O(9)	91.85(11)	O(4)-Ni(1)-N(1)	88.57(12)
O(8)-Ni(1)-N(1)	175.11(13)	O(9)-Ni(1)-N(1)	92.74(13)
O(4)-Ni(1)-O(7)	176.25(12)	O(8)-Ni(1)-O(7)	89.97(11)
O(9)-Ni(1)-O(7)	91.59(11)	N(1)-Ni(1)-O(7)	91.59(12)
O(4)-Ni(1)-N(2)	85.48(12)	O(8)-Ni(1)-N(2)	97.03(12)
O(9)-Ni(1)-N(2)	170.78(12)	N(1)-Ni(1)-N(2)	78.32(13)

O(7)-Ni(1)-N(2)	90.89(12)	O(18)-Ni(2)-N(4)	101.71(12)
O(18)-Ni(2)-O(20)	88.63(12)	N(4)-Ni(2)-O(20)	92.53(14)
O(18)-Ni(2)-N(3)	104.01(12)	N(4)-Ni(2)-N(3)	79.24(14)
O(20)-Ni(2)-N(3)	166.03(13)	O(18)-Ni(2)-O(17)	97.10(11)
N(4)-Ni(2)-O(17)	160.97(11)	O(20)-Ni(2)-O(17)	90.78(12)
N(3)-Ni(2)-O(17)	93.49(12)	O(18)-Ni(2)-O(16)	156.95(11)
N(4)-Ni(2)-O(16)	100.96(11)	O(20)-Ni(2)-O(16)	86.30(11)
N(3)-Ni(2)-O(16)	84.24(11)	O(17)-Ni(2)-O(16)	60.55(9)

STable. 3. Hydrogen bonds for compounds 1 and **2**

D-H	d(D-H)	d (H..A)	<DHA	d (D..A)
compound 1				
O7-H-O3$^{\#1}$	0.820	1.691	164.18	2.490
O11-H-O9$^{\#3}$	0.850	2.044	159.17	2.855
O11-H-Br$^{\#4}$	0.850	2.677	124.61	3.237
O12-H-O3$^{\#5}$	0.850	2.194	156.38	2.992
O12-H-O8$^{\#6}$	0.850	2.019	155.79	2.816
compound 2				
O2-H.....O3$^{\#1}$	0.820	1.765	176.47	2.584
O10-H.....O16$^{\#3}$	0.850	1.928	158.40	2.707
O15-H.....O6$^{\#4}$	0.850	1.886	154.86	2.651
O21-H.....O19$^{\#6}$	0.850	1.840	152.84	2.597

Symmetric code: **Compound 1**:#1 *-x+3, -y+1, -z+2*; #2 *x, y, z-1*; #3 *x-1, y, z* ;#4 *x+1, y+1, z*; #5-*x+1, -y+1, -z+2*;#6 *x-2, y, z*; **Compound 2**:#1 *-x, -y+1, -z-1*; #2 *-x+1, -y+1, -z;* #3*x+1, y+1, z;* #4*x-1, y-1, z;* #5 *-x, -y, -z;* #6 *-x+1, -y, -z+1*

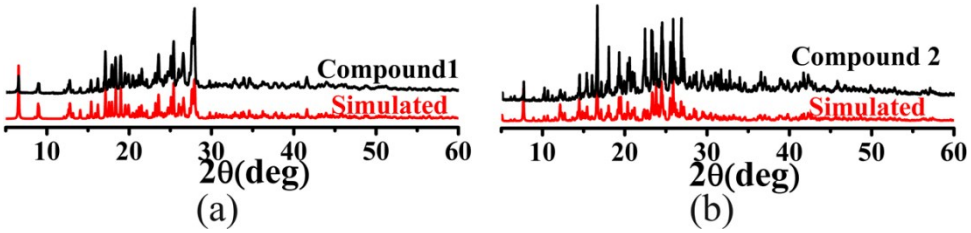

Fig S1. Powder X-ray diffraction patterens of (a) compound 1 and (b) compound 2

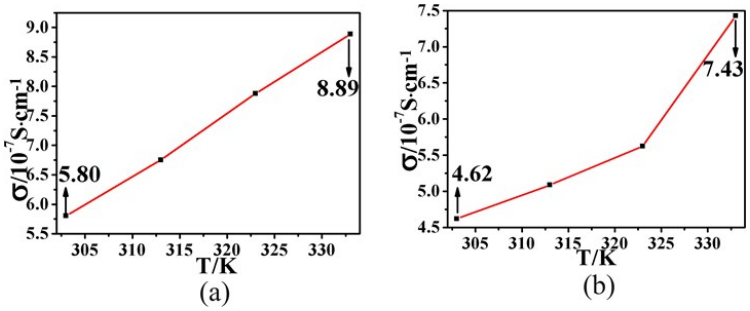

Fig S2. The conductivity **1**/Nafion (a) and **2**/Nafion (b) at different temperature

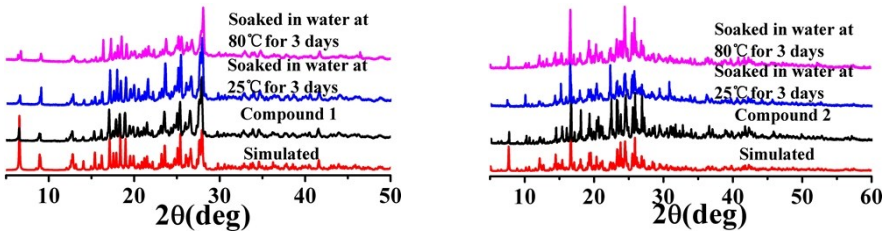

Fig S3. The PXRD patterns of compounds 1 (a) and 2 (b) after water-treatment under different conditions.

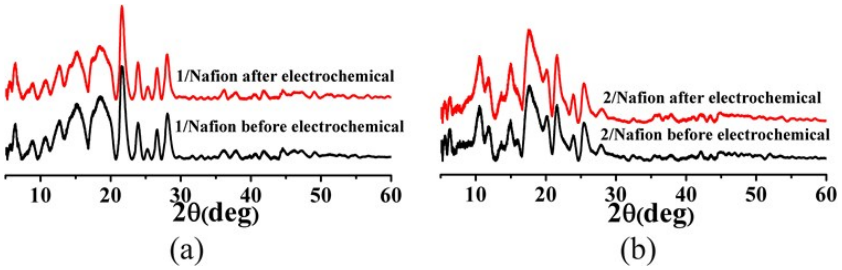

Fig S4. The PXRD patterns of 1/Nafion (a) and 2/Nafion (b) before electrochemical experiment and after electrochemical experiment.

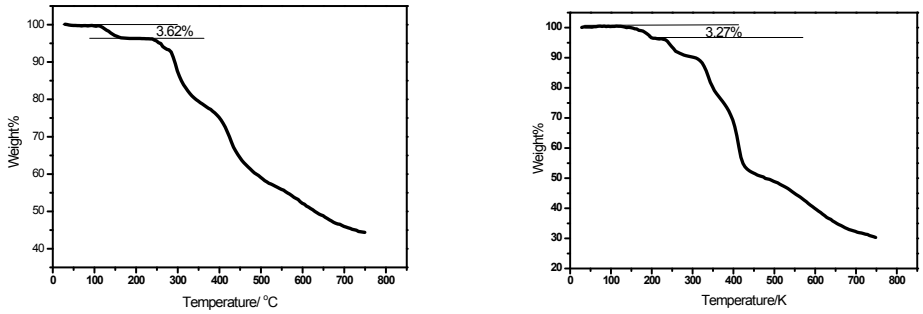

Fig S5. TheTG curves of 1 (a) and 2 (b) .