Supporting Information

High proton conductance in nickel(II) complex and its hybrid membrane

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

	1		
Ni(1)-N(1)	2.106(1)	Ni(1)-N(4)	2.102(1)
Ni(1)-N(2)	2.061(1)	Ni(1)-N(5)	2.086(1)
Ni(1)-N(3)	2.079(1)	Ni(1)-N(6)	2.070(1)
N(2)-Ni(1)-N(1)	78.47(5)	N(5)-Ni(1)-N(3)	169.42(5)
N(3)-Ni(1)-N(1)	98.05(5)	N(5)-Ni(1)-N(4)	92.72(5)
N(3)-Ni(1)-N(2)	93.27(5)	N(6)-Ni(1)-N(1)	92.15(5)
N(4)-Ni(1)-N(1)	176.17(5)	N(6)-Ni(1)-N(2)	168.14(5)
N(4)-Ni(1)-N(2)	100.21(5)	N(6)-Ni(1)-N(3)	95.24(5)
N(4)-Ni(1)-N(3)	78.39(5)	N(6)-Ni(1)-N(4)	89.60(5)
N(5)-Ni(1)-N(1)	90.97(5)	N(6)-Ni(1)-N(5)	78.81(5)
N(5)-Ni(1)-N(2)	93.96(5)	C(1)-N(1)-Ni(1)	127.28(1)

Table S2. Hydrogen bond lengths (Å) and angles (°) for **1.**

		1		
D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
O(2)-H(2A)…O(6a)	0.82	1.64	2.431(1)	162
O(4)-H(4A)…O(13b)	0.82	1.77	2.591(2)	176
O(10)-H(10B)…O(7c)	0.83(1)	2.29(2)	2.998(1)	144(2)
O(11)-H(11A)…O(9d)	0.86(3)	2.13(3)	2.934(2)	156(2)
O(11)-H(11B)…O(8)	0.87(1)	2.07(1)	2.923(1)	165(3)
O(12)-H(12A)…O(5e)	0.86(2)	1.98(2)	2.839(2)	171(2)
O(13)-H(13A)…O(14f)	0.85(2)	2.22(2)	3.051(2)	165(2)
O(13)-H(13A)…O(3)	0.85(2)	2.56(2)	3.121(2)	125(2)
O(13)-H(13B)…O(12g)	0.85(2)	1.94(3)	2.775(2)	167(2)
O(14)-H(14A)…O(3h)	0.86(2)	2.02(2)	2.754(2)	144(2)
O(14)-H(14B)…O(8i)	0.87(2)	2.03(2)	2.902(1)	176(2)
C(7)-H(7)…O(1j)	0.93	2.34	3.134(1)	143
C(9)-H(9)…O(5k)	0.93	2.58	3.188(2)	123

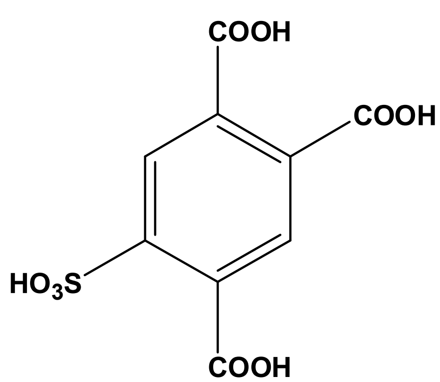
Symmetry codes: a) -x+1/2, y-1/2, -z+1/2; b) -x+1, -y+2, -z; c) -x, -y+1, -z+1; d) –x+1, -y+1, -z; e) x, y-1, z; f) x, y, z-1; g) x, y+1, z; h) x, y, z+1; i) –x+1, -y+1, -z+1; j) x+1, y, z; k) x+1, y-1, z.

Table S3. Proton conduction performances at high RH of some selected coordination compounds

Selected coordination compound	Conductivity ($S \cdot cm^{-1}$)	Measurement condition	Ea (ev)	Ref
$[Ni(2,2'\text{-}bpy)_4](H_2SBTC)(H_2O)_5$	1.3×10^{-4}	313K, 98%RH	0.17	our work
$[Cu(bipy)_2(1,4\text{-}BDMS)(H_2O)_{0.5}]_n$	1.2×10^{-4}	363K, 98%RH	0.37	1
$\{[Cu(pyz)(5\text{-}Hsip)(H_2O)_2]\cdot(H_2O)_2\}_n$	3.5×10^{-5}	338K, 95%RH	0.35	2
$Zn_3(IBT)_2(H_2O)_2$	2.1×10^{-5}	308K, 97%RH	0.14	3
$Cu(H_2spip)Cl_2\cdot H_2O$	1.1×10^{-2}	368K, 97%RH	0.19	4
$K_2(H_2adp)[Zn_2(ox)_3]\cdot 3H_2O$	1.2×10^{-4}	298K, 98%RH	0.45	5
MFM-500(Ni)	4.5×10^{-4}	298K, 98%RH	0.43	6
$[\{In_2(\mu\text{-}OH)_2(SO_4)_4\}\cdot\{(LH)_4\}\cdot nH_2O]_n$	4.4×10^{-5}	303K, 98%RH	0.32	7

Table S4. Proton conduction properties of some selected coordination compound composite membranes

Selected MOF composite membranes	Conductivity ($S \cdot cm^{-1}$)	Measurement condition	Ea (ev)	Ref
1@PVA-5	1.6×10^{-3}	313K, 98% RH	0.78	our work
MOF-508@PVDF-55	1.56×10^{-4}	338K, 100% RH	0.17	8
JUC-200@PVA-10	1.3×10^{-3}	323K, 100% RH	0.46	9
Ca-MOF@PVP-50	5.7×10^{-5}	298K, 65% RH	0.54	10
S-MIL-101@CS-4	6.4×10^{-2}	373K,100% RH	0.17	11
S-UiO-66@GO@SPEEK-10	2.7×10^{-1}	343K, 95% RH	0.10	12



Scheme S1. Structure of H_4SBTC ligand.

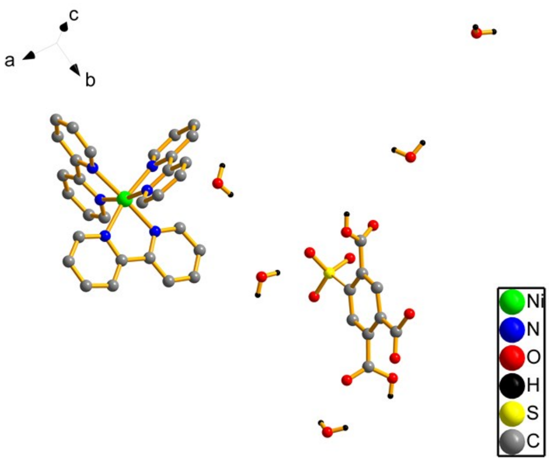


Fig. S1 Single cell diagram of **1.**

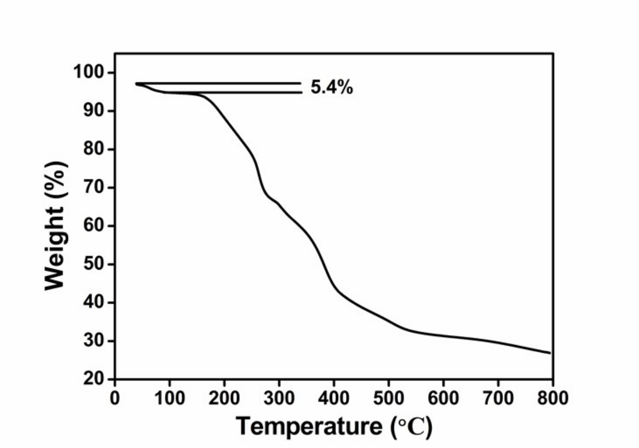


Fig. S2 TGA curve of **1**.

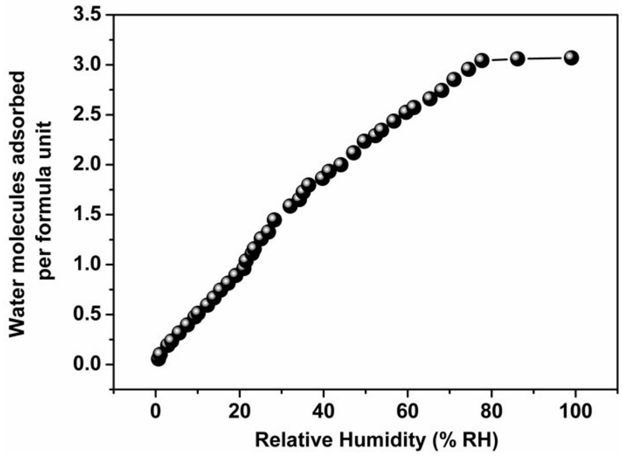


Fig. S3 Water vapor adsorption isotherms of **1** (at 25℃).

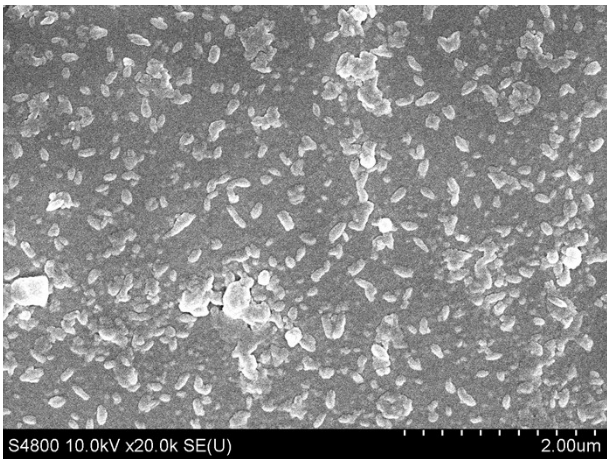


Fig. S4 The SEM image shows the surfaces of the **1**@PVA-8 composite membrane.

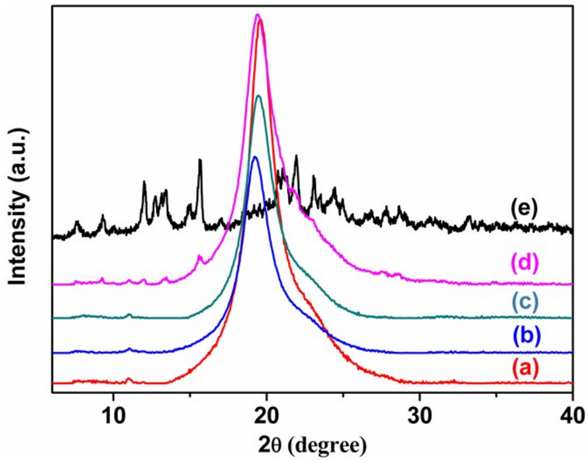


Fig. S5 PXRD patterns of pure PVA, 1@PVA composite membranes and **1** ((a) pure PVA, (b) **1**@PVA-3, (c) **1**@PVA-5, (d) **1**@PVA-8, (e) **1**).

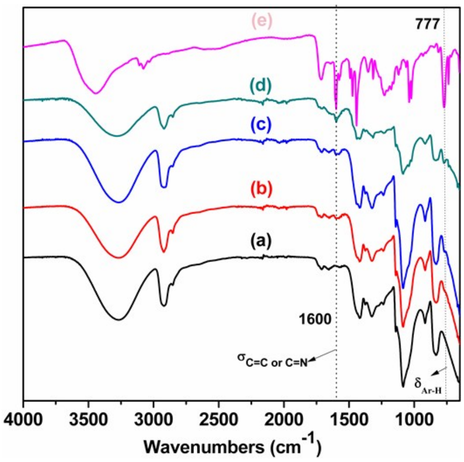


Fig. S6 FTIR spectra of pure PVA, the composite membranes and **1** ((a) pure PVA, (b) **1**@PVA-3, (c) **1**@PVA-5, (d) 1@PVA-8, (e) **1**).

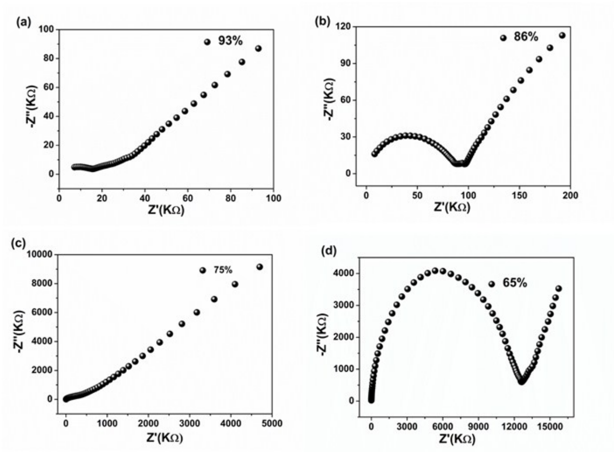


Fig. S7 Nyquist plots of **1** under different relative humidity at 298 K.

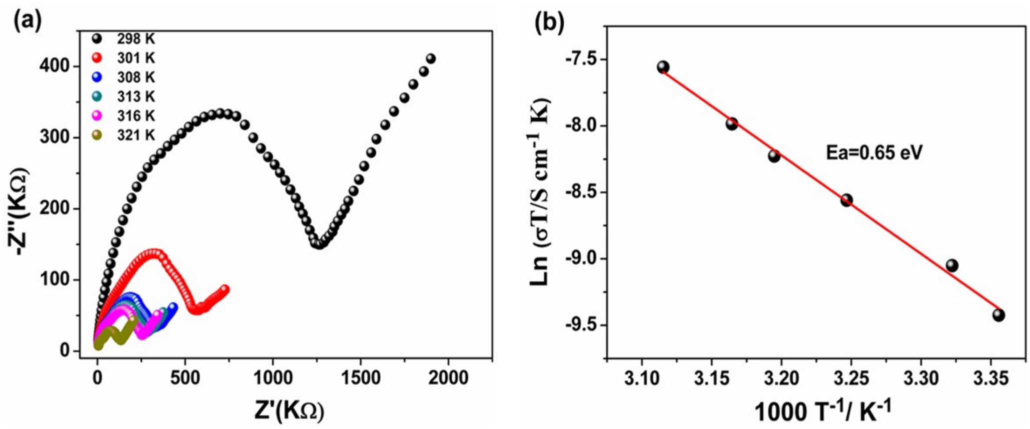


Fig. S8 (a) Nyquist plots of PVA at different temperature and 98% RH; (b) Arrhenius plot of Ln(σT) against 1000/T of PVA under 98% RH, the red solid line represents the best fit of the date from 298 K to 321 K.

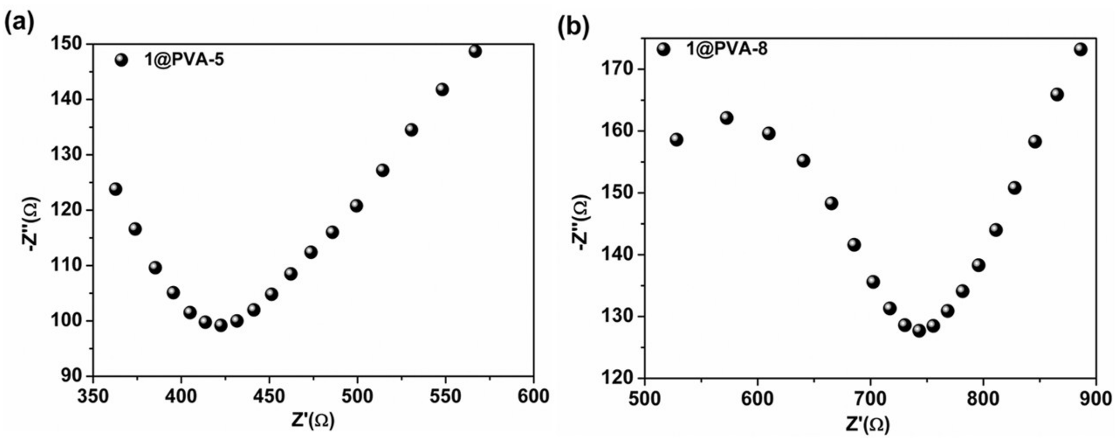


Fig.S9 Nyquist plot of 1@PVA-5 (a) and 1@PVA-8 (b) at 298 K under 98% RH.

References

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