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Supporting Information

A water stable Ni(II) diphosphonate exhibiting water vapor adsorption and water-assisted high proton conductivity

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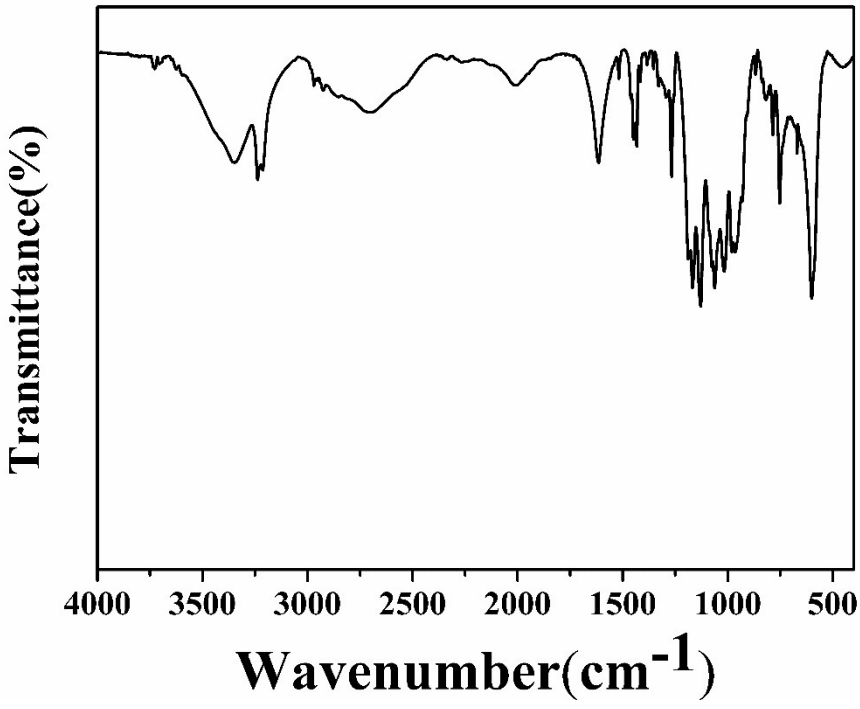

Figure S1. The IR spectrum of **1**.

Table S1. Crystallographic data for complex 1

	1
CCDC No.	1812311
Empirical formula	$C_{18}H_{50}N_2O_{26}P_4F_2Ni_3$
Formula weigh	1048.55
T/K	293
Crystal system	monoclinic
Space group	P 21/c

a/Å	19.126(2)
b/Å	6.2821(6)
c/Å	15.7341(18)
α^o	90
$\beta/^o$	106.417(4)
$\gamma/^o$	90
V/Å^3	1813.4(3)
Z	2
D_{calc}/g cm^{-3}	1.920
μ/mm^{-1}	1.828
F(000)	1084.0
h, k, l max	23, 7, 18
S	1.037
R_1, wR_2 [I> 2σ(I)]	0.0488, 0.0929

Table S2. Selected bond lengths (Å) and bond angles (^{o}) for complex 1

Complex **1**					
Ni1-O3	2.020(4)	O3^i-Ni1-O2	175.67(17)	O8-Ni1-O7	90.44(16)
Ni1-O2	2.066(4)	O3^i-Ni1-O8	91.58(15)	O4-Ni1-O7	175.20(15)
Ni1-O8	2.090(4)	O2-Ni1-O8	89.17(15)	O3^i-Ni1-N1	94.00(17)
Ni1-O4	2.2099(4)	O3^i-Ni1-O4	88.08(15)	O2-Ni1-N1	85.69(15)
Ni1-O7	2.103(4)	O2-Ni1-O4	96.21(15)	O8-Ni1-N1	172.01(17)

Ni1-N1	2.191(4)	O8-Ni1-O4	87.92(15)	O4-Ni1-N1	86.56(15)
		$O3^{i}$-Ni1-O7	87.45(15)	O7-Ni1-N1	85.51(16)
		O2-Ni1-O7	88.28(15)		

Table S3. Hydrogen bonds parameters of complex 1.

Donor atom	H atom	Acceptor atom	Distance D-H	Distance H-A	Distance D-A	Angle D-H-A
O13	H13B	O12	0.8500	2.0600	2.868(6)	159.000
O13	H13A	O8	0.8500	2.1900	2.689(6)	117.100
O13	H13A	O2	0.8500	2.2900	3.101(6)	159.200
O12	H12B	O10	0.8500	2.3300	3.174(6)	175.700
O12	H12A	O6	0.8500	1.9400	2.788(6)	176.500
O11	H11B	O5	0.8500	1.9800	2.808(5)	164.200
O11	H11A	O3	0.8500	2.3100	3.139(6)	164.600
O10	H10B	O12	0.8500	2.6200	3.174(6)	123.700
O10	H10B	O8	0.8500	2.6400	3.416(5)	152.700
O10	H10A	O8	0.8500	2.5500	3.338(5)	154.900
O10	H10A	O2	0.8500	2.1700	2.714(5)	121.600
O9	H9D	O8	0.8500	2.1800	2.964(6)	152.600
O8	H8D	O9	0.8500	2.1900	2.964(6)	150.500
O8	H8D	O4	0.8500	2.5000	2.908(5)	110.800
O8	H8C	O13	0.8500	2.0500	2.689(6)	131.900

O8	H8C	O10	0.8500	2.6000	3.338(5)	145.900
O7	H7D	O6	0.8500	2.2000	3.032(5)	164.800
O7	H7C	O5	0.8500	2.0100	2.773(5)	148.600
O6	H6A	O12	0.8500	2.3300	2.788(6)	113.700
O6	H6A	O11	0.8500	2.5400	3.368(5)	164.100
O1	H1A	O7	0.8500	2.5800	3.377(5)	157.200