Proton conduction studies on four porous and nonporous coordination polymers with different acidity and water uptake

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Table S1 the selected bond lengths and angels of compounds **1**-**4**.

1			
Cd(1)-O(1)	2.214(5)	Cd(1)-O(2)#1	2.250(5)
Cd(1)-O(3)	2.288(8)	Cd(1)-O(4)	2.321(8)
Cd(1)-O(5)#2	2.346(5)	Cd(1)-O(6)#2	2.368(5)
O(1)-Cd(1)-O(2)#1	124.7(2)	O(1)-Cd(1)-O(3)	89.4(3)
O(2)#1-Cd(1)-O(3)	89.7(3)	O(1)-Cd(1)-O(4)	87.7(3)
O(2)#1-Cd(1)-O(4)	87.6(2)	O(3)-Cd(1)-O(4)	174.0(3)
O(1)-Cd(1)-O(5)#2	94.99(19)	O(2)#1-Cd(1)-O(5)#2	140.33(19)
O(3)-Cd(1)-O(5)#2	90.2(3)	O(4)-Cd(1)-O(5)#2	95.3(2)
O(1)-Cd(1)-O(6)#2	149.7(2)	O(2)#1-Cd(1)-O(6)#2	85.46(18)
O(3)-Cd(1)-O(6)#2	94.2(3)	O(4)-Cd(1)-O(6)#2	91.0(3)
O(5)#2-Cd(1)-O(6)#2	54.99(16)		
2			
Ni(1)-O(2)	2.097(6)	Ni(1)-O(7)#1	2.040(6)
Ni(1)-O(11)	2.052(5)	Ni(1)-O(12)	2.087(6)
Ni(1)-N(3)	2.048(6)	Ni(1)-N(4)	2.079(7)
Ni(2)-O(1)	2.020(5)	Ni(2)-O(4)#2	2.022(6)
Ni(2)-O(5)#3	2.178(6)	Ni(2)-O(6)#3	2.097(5)
Ni(2)-N(1)	2.097(7)	Ni(2)-N(2)	2.068(6)
O(7)#1-Ni(1)-N(3)	84.3(2)	O(7)#1-Ni(1)-O(11)	92.4(2)
N(3)-Ni(1)-O(11)	171.1(3)	O(7)#1-Ni(1)-N(4)	97.4(2)
N(3)-Ni(1)-N(4)	79.1(3)	O(11)-Ni(1)-N(4)	93.2(2)
O(7)#1-Ni(1)-O(12)	88.3(2)	N(3)-Ni(1)-O(12)	98.9(2)
O(11)-Ni(1)-O(12)	89.2(2)	N(4)-Ni(1)-O(12)	173.8(3)
O(7)#1-Ni(1)-O(2)	169.9(2)	N(3)-Ni(1)-O(2)	87.3(2)
O(11)-Ni(1)-O(2)	96.8(2)	N(4)-Ni(1)-O(2)	86.4(3)
O(12)-Ni(1)-O(2)	87.6(2)	O(1)-Ni(2)-O(4)#2	89.3(2)

O(1)-Ni(2)-N(2)	88.8(2)	O(4)#2-Ni(2)-N(2)	97.9(3)
O(1)-Ni(2)-O(6)#3	100.4(2)	O(4)#2-Ni(2)-O(6)#3	99.0(2)
N(2)-Ni(2)-O(6)#3	160.8(3)	O(1)-Ni(2)-N(1)	166.1(3)
O(4)#2-Ni(2)-N(1)	97.4(3)	N(2)-Ni(2)-N(1)	78.3(3)
O(6)#3-Ni(2)-N(1)	90.6(2)	O(1)-Ni(2)-O(5)#3	88.9(2)
O(4)#2-Ni(2)-O(5)#3	159.9(2)	N(2)-Ni(2)-O(5)#3	102.1(2)
O(6)#3-Ni(2)-O(5)#3	61.7(2)	N(1)-Ni(2)-O(5)#3	88.9(3)
3			
Ni(1)-N(1)	2.058(4)	Ni(1)-O(5)	2.090(4)
Ni(1)-O(4)	2.136(3)	Ni(2)-N(2)	2.133(4)
Ni(2)-O(7)	2.080(4)	Ni(2)-O(8)	2.031(3)
N(1)#1-Ni(1)-N(1)	180.0	N(1) -Ni(1)-O(5)	88.97(16)
N(1)-Ni(1)-O(5)#1	91.03(16)	O(5)#1-Ni(1)-O(5)	180.00(12)
N(1)-Ni(1)-O(4)	89.74(16)	N(1)-Ni(1)-O(4)#1	90.26(16)
O(5) -Ni(1)-O(4)	62.49(14)	O(5)-Ni(1)-O(4)#1	117.51(14)
N(1)#1-Ni(1)-O(4)	90.26(16)	O(4)#1-Ni(1)-O(4)	180.0 (2)
O(8)-Ni(2)-O(8)#2	180.0(4)	O(8)-Ni(2)-O(7)#2	86.93(14)
O(8)-Ni(2)-O(7)	93.07(14)	O(7)#2-Ni(2)-O(7)	180.0
O(8)-Ni(2)-N(2)	90.03(15)	O(8)#2-Ni(2)-N(2)	89.97(15)
O(7)#2-Ni(2)-N(2)	89.36(16)	O(7)-Ni(2)-N(2)	90.64(16)
N(2)-Ni(2)-N(2)#2	180.04		
4			
Co(1)-O(1)	2.1444(19)	Co(1)-O(2)	2.0548(19)
Co(1)-N(1)	2.214(2)		
O(2)#1-Co(1)-O(2)	180.00(10)	O(2)#1-Co(1)-O(1)#1	89.94(8)
O(2)-Co(1)-O(1)#1	90.06(8)	O(2)-Co(1)-O(1)	89.94(8)
O(1)#1-Co(1)-O(1)	180.0	O(2)#1-Co(1)-N(1)	86.46(8)
O(2)-Co(1)-N(1)	93.54(8)	O(1)#1-Co(1)-N(1)	93.52(8)
O(1)-Co(1)-N(1)	86.48(8)	N(1)-Co(1)-N(1)#1	180.0

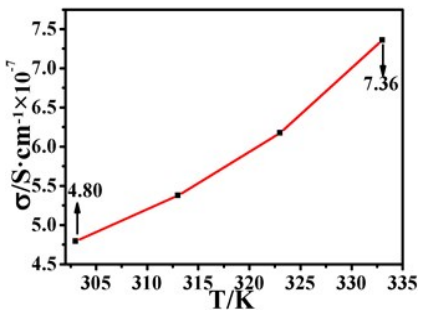
Symmetry transformations used to generate equivalent atoms: **1** #1 -x, -y+1, -z+1; #2 -x-1/2, -y+3/2, -z+1; **2** #1 x-1, y+1, z-1; #2 x-1, y, z; #3 -x+1, -y+2, -z+2; **3** #1 -x+3, -y+1, -z+1; #2 -x+1, -y, -z; **4** #1 -x+3/2, -y+1/2, -z+1.

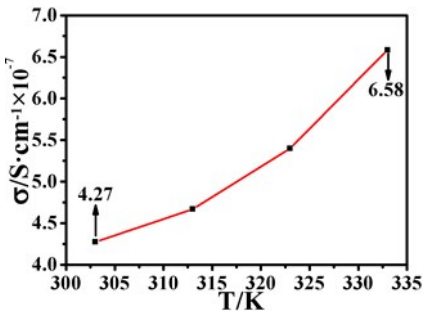
Table S2 The hydrogen bond parameters of compounds **1-4**.

D-H	d(D-H)	d(H···A)	<DHA	d(D···A)

1				
O3-H···O2^{i}	0.850	2.393	132.35	3.032
O3-H···O6^{ii}	0.850	1.843	163.78	2.670
O4-H···O7^{iii}	0.850	2.326	115.63	2.801
O4-H···O8^{iv}	0.850	2.352	131.79	2.987
O8-H···O3^{v}	0.850	1.896	149.61	2.665
O8-H···O4	0.850	2.484	165.70	3.314
2				
O9-H···O4^{i}	0.850	1.848	173.62	2.694
O9-H···O7^{ii}	0.850	2.205	136.27	2.880
O10-H···O15^{iii}	0.850	2.059	145.06	2.798
O10-H···O6^{ii}	0.850	2.014	152.25	2.794
O11-H···O16^{iv}	0.850	1.940	175.55	2.789
O11-H···Br4^{v}	0.850	2.498	158.44	3.303
3				
O1-H···O7^{i}	0.820	1.982	150.54	2.726
O7-H···O13^{ii}	0.850	1.982	141.28	2.698
O7-H···O9	0.850	2.024	130.65	2.657
O11-H···O4^{iii}	0.820	1.866	161.52	2.656
O13-H···O9^{iv}	0.850	2.035	173.23	2.881
O13-H···O10^{v}	0.850	2.130	173.38	2.976
4				
O1-H···O5^{i}	0.850	2.140	151.93	2.917
O1-H···O3	0.850	2.019	142.78	2.745
O4-H···O3^{ii}	0.820	1.802	151.10	2.551

Symmetry codes: **1**: i x - 1, y, z; ii x - 1/2, y - 1/2, z; iii -x + 1/2, -y + 3/2, -z + 1; iv -x, y, -z+1/2; v -x, -y + 1, -z + 1; **2**: i -x + 1, -y + 1, -z; ii x + 1, y, z; iii x + 1, y - 1, z + 1; iv -x, -y + 2, -z; v -x + 1, -y + 2, -z; **3**: i -x + 2, -y, -z + 1; ii x, y - 1, z – 1; iii x - 1, y, z – 1; iv -x, -y + 1, -z + 1; v x, y, z + 1; **4**: i x, y - 1, z; ii -x + 3/2, y + 1/2, -z + 3/2.





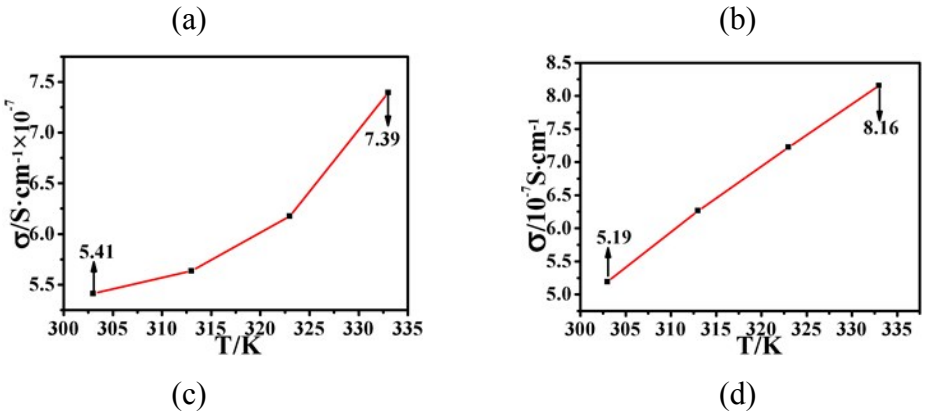


Figure S1 The proton conductivities of compounds **1**(a), **2**(b), **3**(c) and **4**(d) at different temperature.