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Iron(III) identification and proton conduction of a luminescent metal-organic framework

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Supporting Information

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Table S1 Selected bond distances (Å) and angles (deg) for compound **1**.

Cd1-O1	2.329(4)	Cd1-N4#1	2.307(5)
Cd1-N1	2.330(5)	Cd1-O15#1	2.413(5)
Cd1-O5	2.227(5)	Cd1-O17	2.246(5)
N1-Cd1-O1	72.69(17)	O15#1-Cd1-O5	83.17(16)
O5-Cd1-O1	63.72(5)	O4-Sr1-O1#5	96.81(5)
O5-Cd1-N1	104.26(17)	O17-Cd1-O1	87.92(18)
N4#1-Cd1-O1	123.88(17)	O17-Cd1-N1	150.13(19)
N4#1-Cd1-N1	82.22(19)	O17-Cd1-O5	95.41(18)
N4#1-Cd1-O5	152.69(17)	O17-Cd1-N4#1	90.6(2)
O15#1-Cd1-O1	165.22(15)	O17-Cd1-O15#1	88.10(18)
O15#1-Cd1-N1	116.07(18)		

Symmetry transformations used to generate equivalent atoms for **1**:#1: 1+X, +Y, +Z; #2: -1+X, +Y, +Z.

Table S2 Hydrogen bonding parameters for **1**.

D-H...A	**d(D-H)**	**d(H...A)**	**d(D...A)**	**∠(DHA)**
O3-H3...O2	0.82	1.66	2.462(6)	164.9
O14-H14...O6	0.82	1.64	2.446(6)	167.6
O17-H17A...O6#3	0.85	1.96	2.731(6)	151
O7-H17B...O15#4	0.85	1.95	2.773(6)	161.4

Symmetry codes: #3: -X, Y+1/2, -Z+3/2; #4: -X+1, Y+1/2, -Z+3/2.

Table S3 A comparison of the Stern-Volmer constant (Ksv), detection limits for Fe^{3+} detection for MOFs/CPs reported in references.

Compounds	Solvents	Ksv / M^{-1}	Detection Limit/ M	Ref.
Tb(3+)@Zn-MOF	ethanol	1.57×10^{4}	7.5×10^{-6}	1
{[Zn3(mtrb)3(btc)2]·3H20n	water	$6.50\times10^{3}M^{-1}$	1.78×10^{-6}	2
CDs	water	-	0.239×10^{-6}	3
Tb-DSOA	water	3.54×10^{3}	-	4
EuL_3	water	4.10×10^{3}	5×10^{-4}	5
[Me2NH2][Eu(CPA)2(H2O)2]	water	1.04×10^{4}	10^{-7}	6
$[Cd(p\text{-CNPhHIDC})(4,4'\text{-bipy})_{0.5}]_n$	water	1.99×10^{3}	5×10^{-3}	7
$[Zn(p\text{-CNPhHIDC})(4,4'\text{-bipy})]_n$	water	1.37×10^{3}	5×10^{-3}	7
1	water	7.16×10^{2}	3.98×10^{-6} M	This work

References

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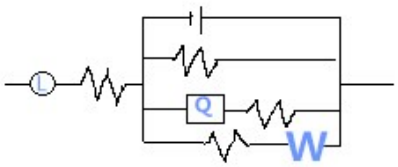
Equivalent circuit LR(CR(QR)(RW)):



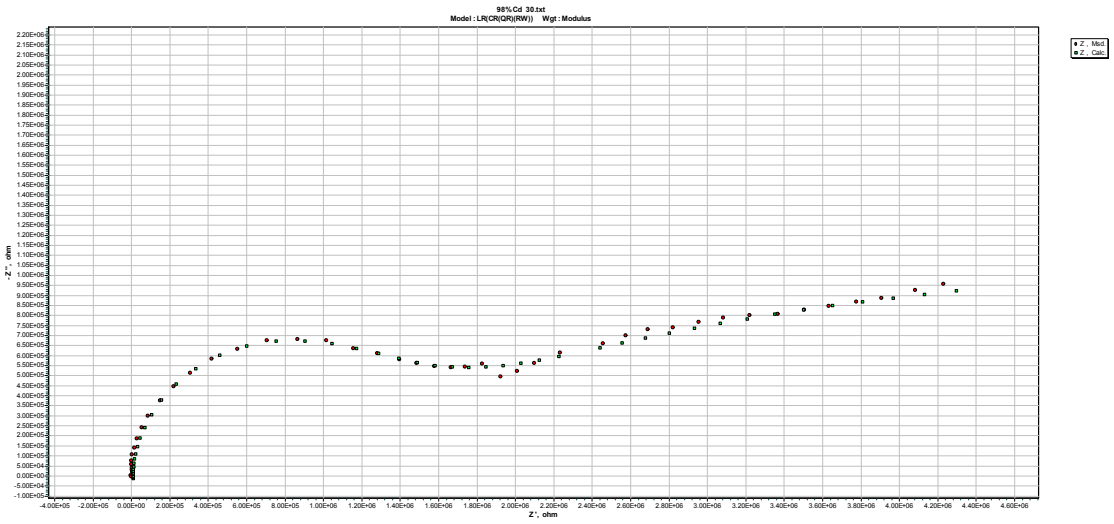


Fig. S1 Nyquist plots for a polycrystalline sample of **1** at 30℃ and 98% RH. Red circle and green square are the measured impedance spectroscopy values and the fits of the impedance data to the equivalent circuit of LR(CR(QR)(RW)).

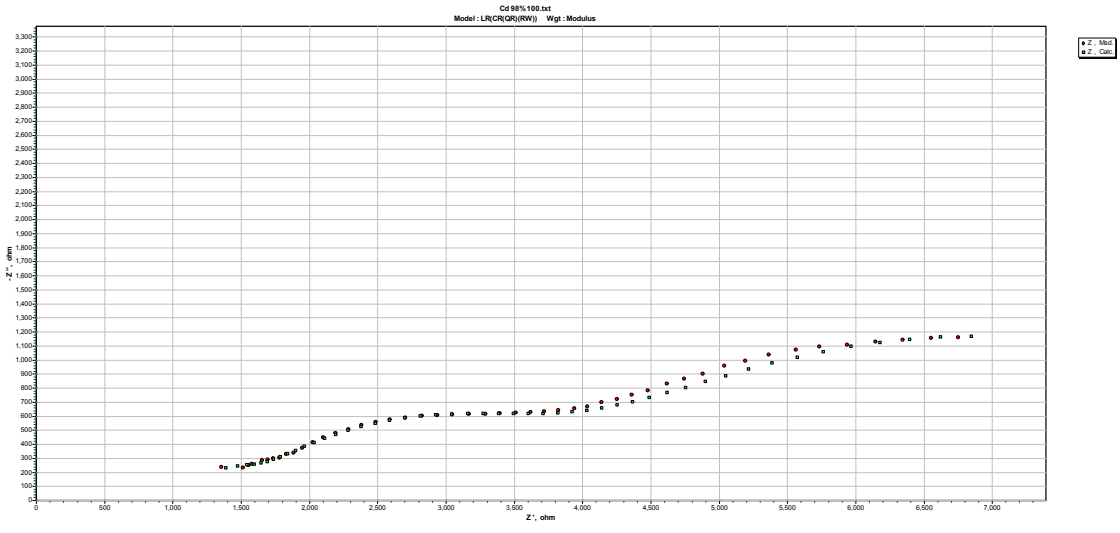


Fig. S2 Nyquist plots for a polycrystalline sample of **1** at 100℃ and 98% RH. Red circle and green square are the measured impedance spectroscopy values and the fits of the impedance data to the equivalent circuit of LR(CR(QR)(RW)).

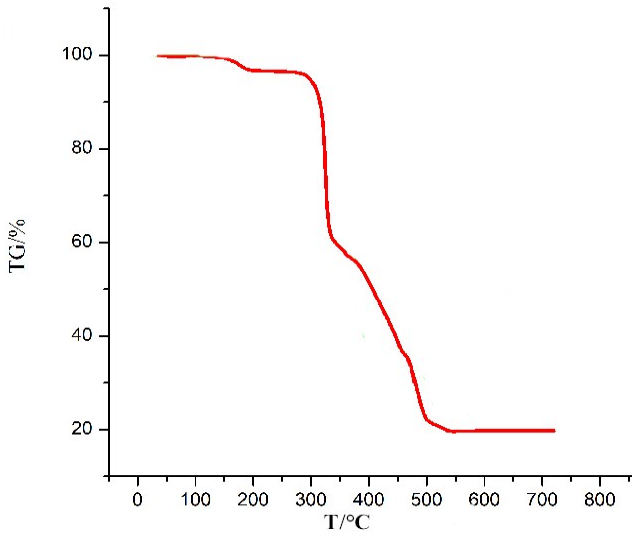


Fig. S3 The TG curve of MOF **1**.

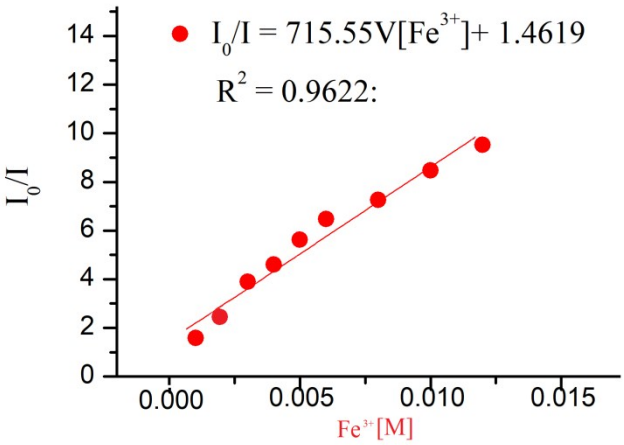


Fig. S4 Stern–Volmer plot of **1** quenched by Fe^{3+}.

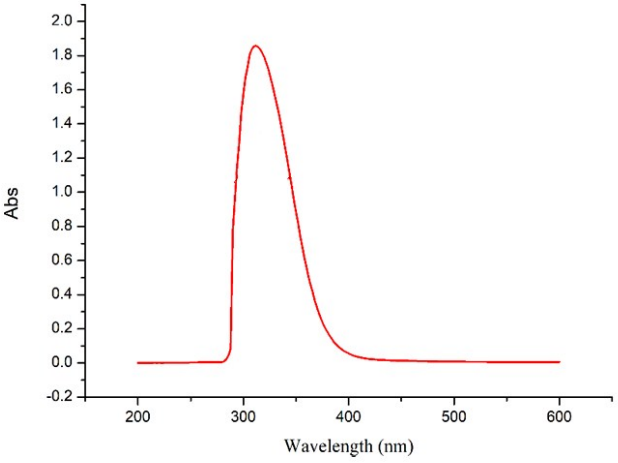


Fig. S5 The liquid UV-Vis spectrum of pure $Fe(NO_3)_3$.

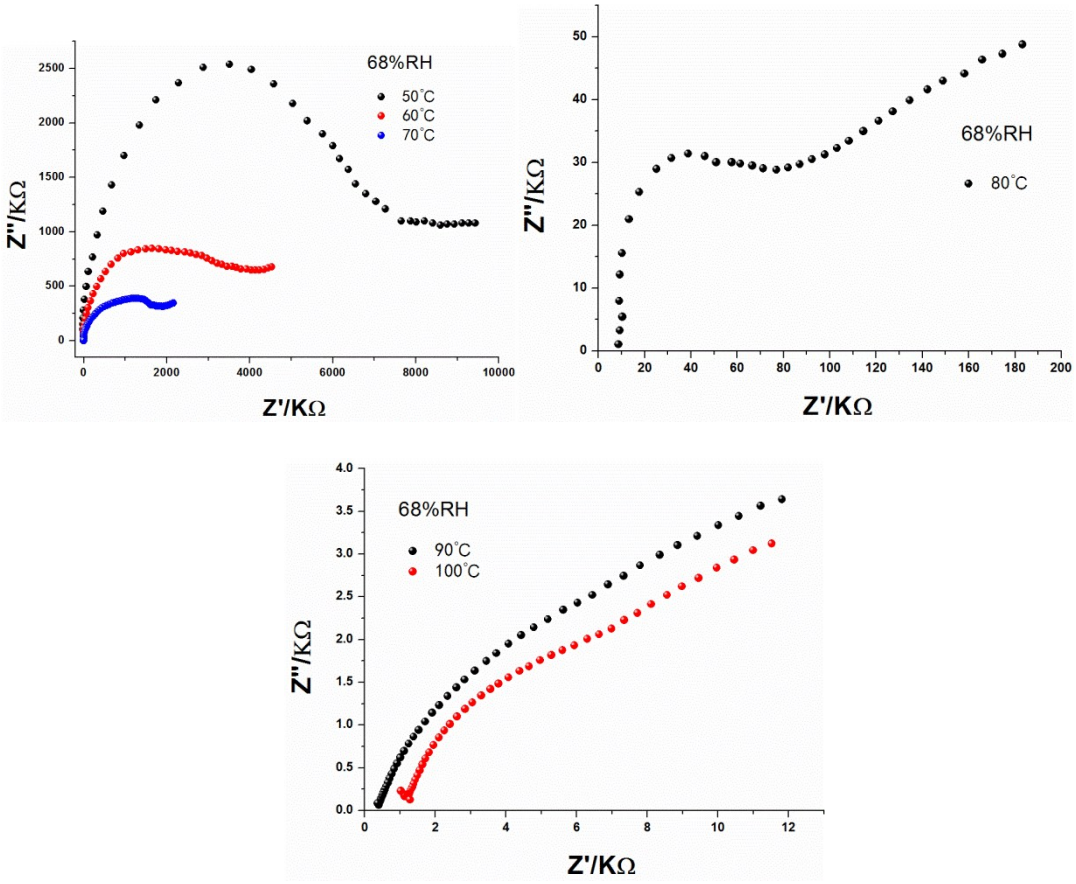


Fig. S6 Impedance spectra of **1** from 50-100 °C at 65% RH.

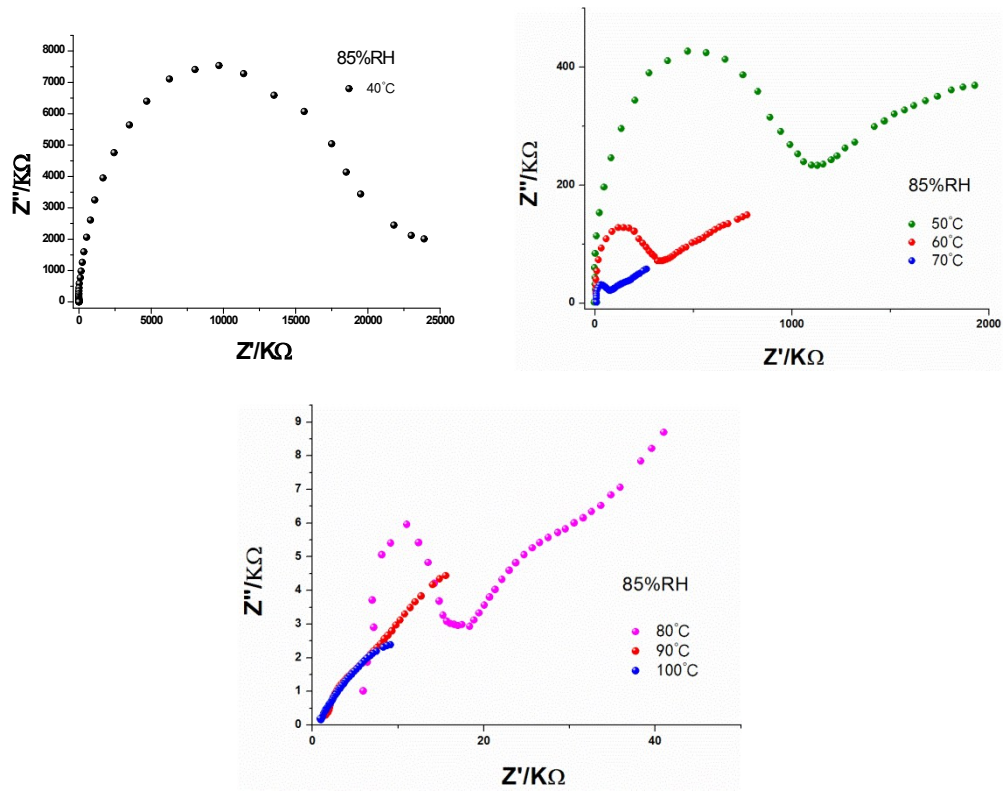


Fig. S7 Impedance spectra of **1** from 40-100 °C at 85% RH.

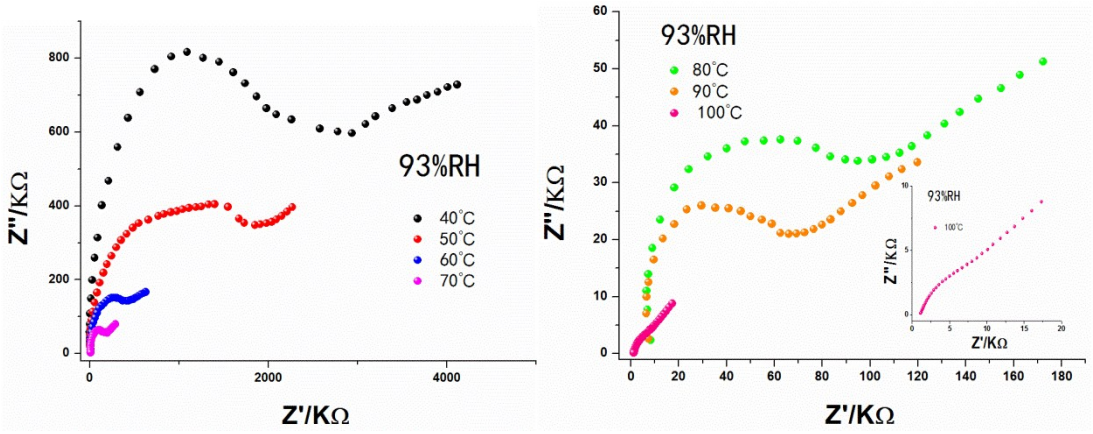


Fig. S8 Impedance spectra of **1** from 40-100 °C at 93% RH.