# High proton conductivity behavior in a 2D metal sulfite constructed from a histidine ligand

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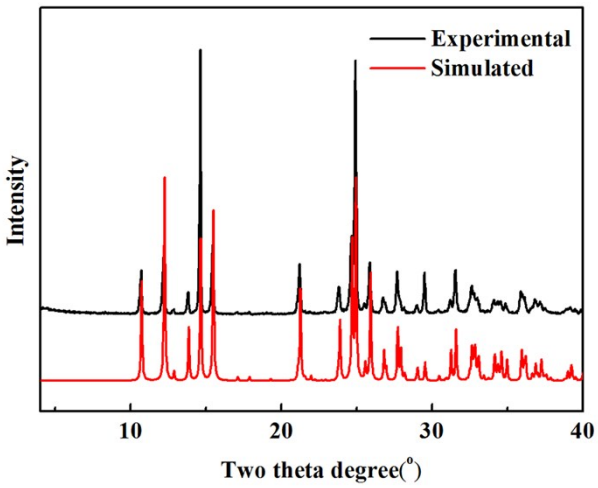


**Fig. S1** Simulated and experimental power X-ray diffraction patterns.

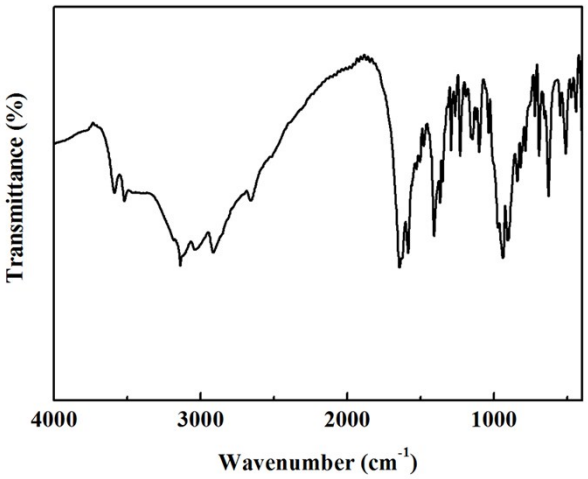


**Fig. S2** The IR spectrum of compound **1**.

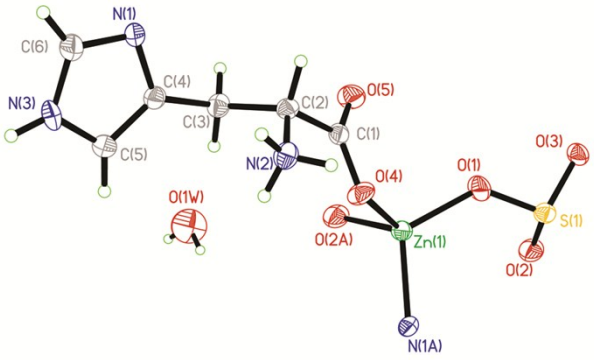


**Fig. S3** The asymmetric unit structure of compound **1**.

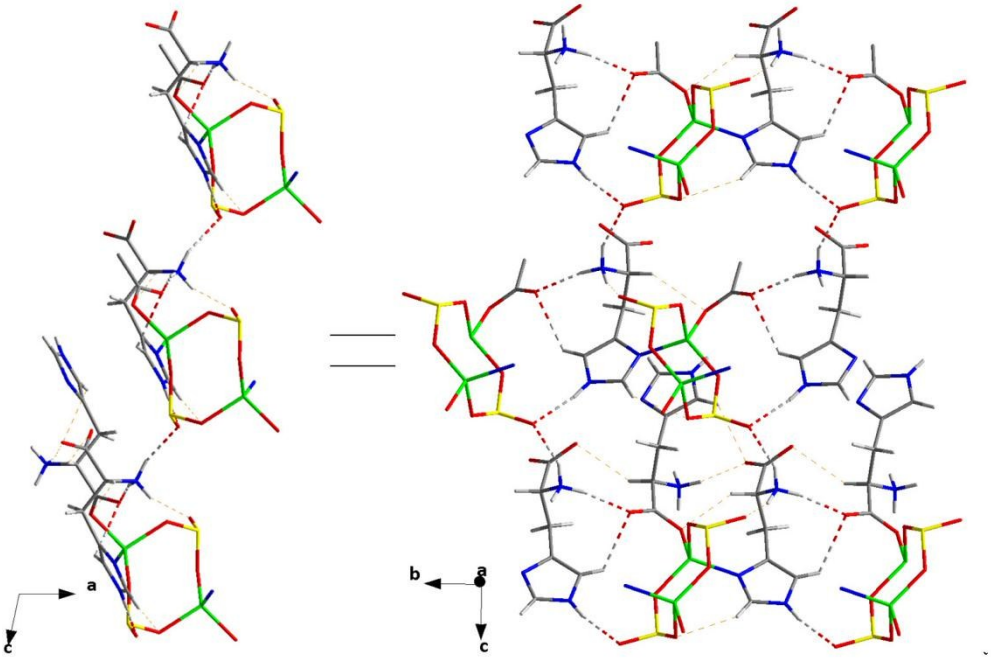


**Fig. S4** View of the 1D H-bonding array between the between histidine molecules and sulfite groups.

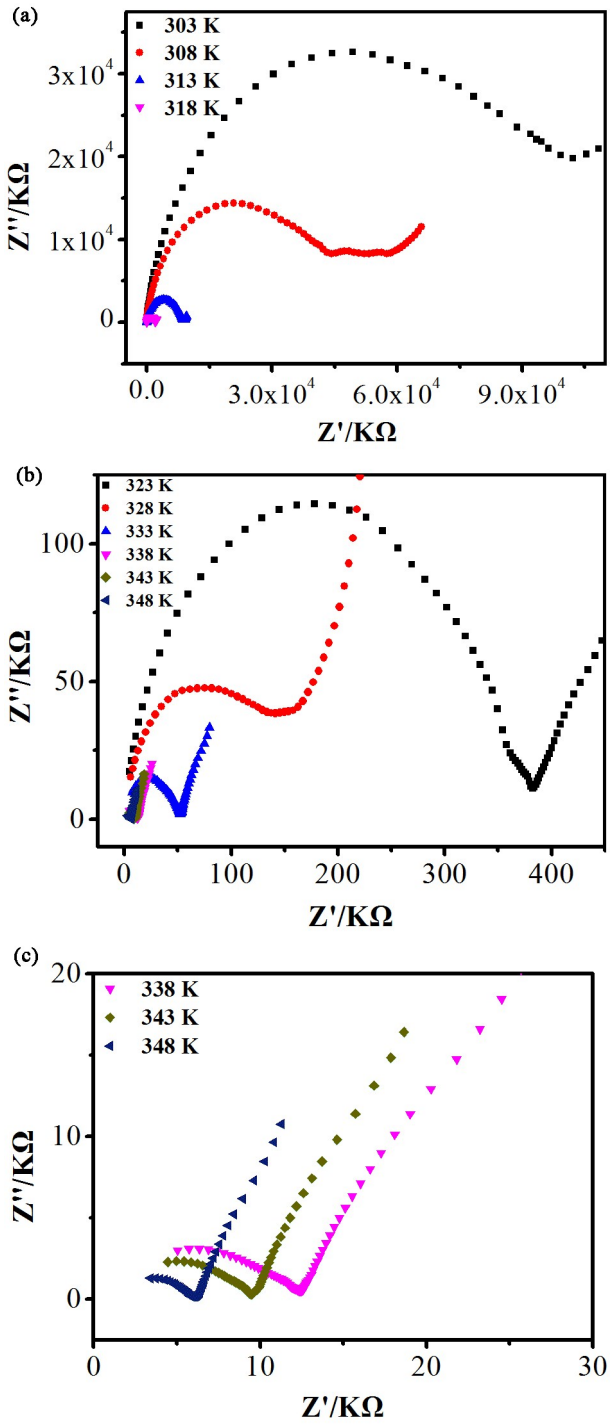


**Fig. S5** Nyquist plots at various temperatures at 44 % RH.

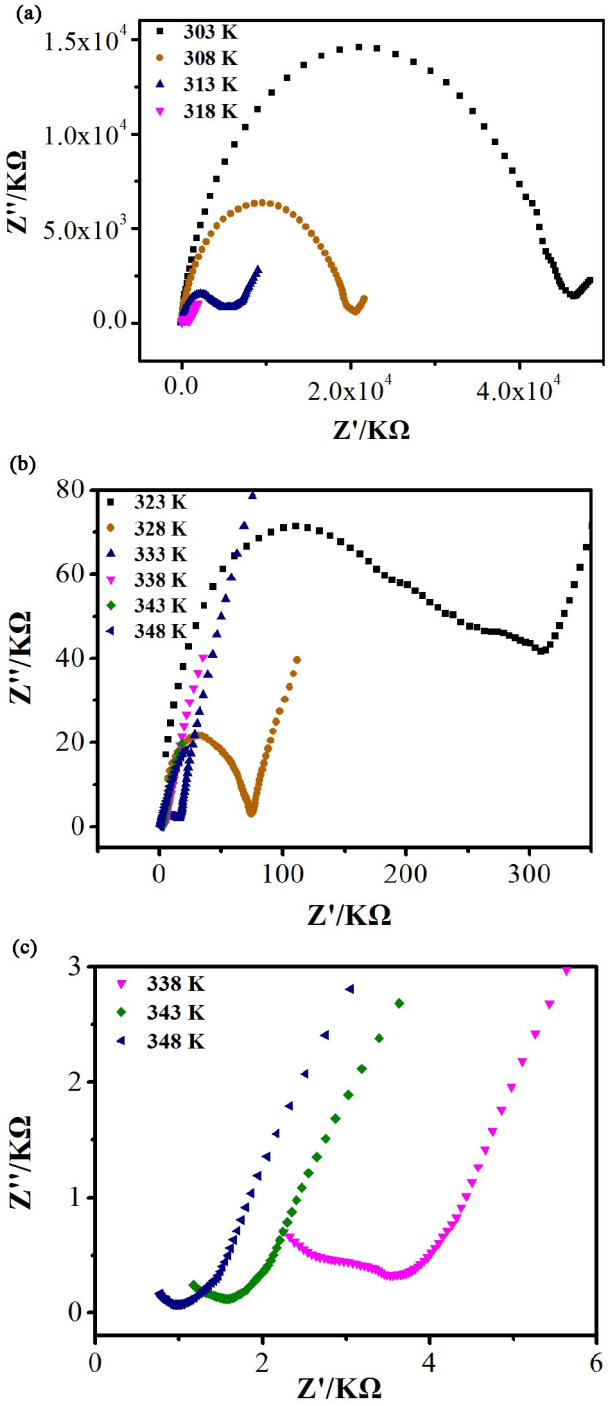


**Fig. S6** Nyquist plots at various temperatures at 58 % RH.

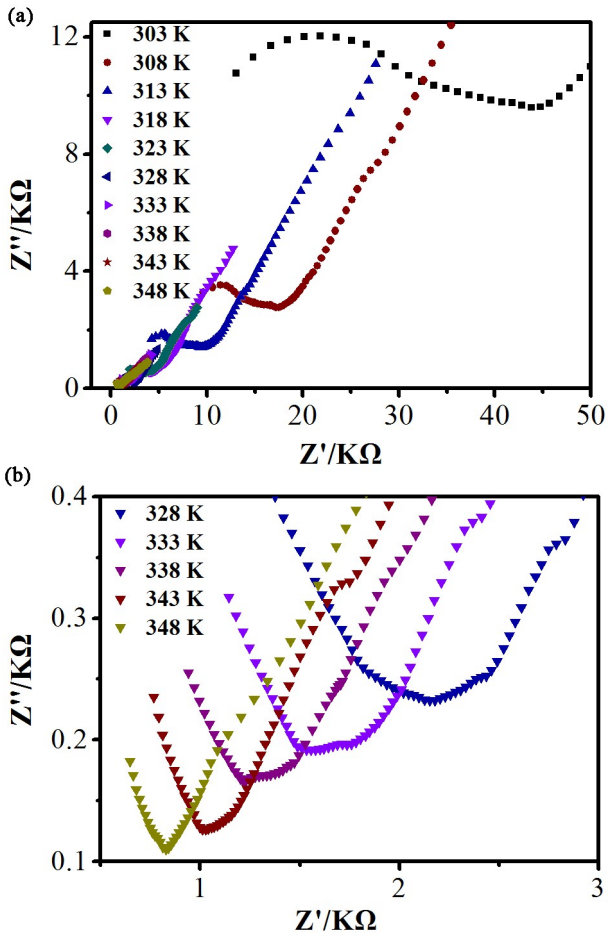


**Fig. S7** Nyquist plots at various temperatures at 76 % RH.

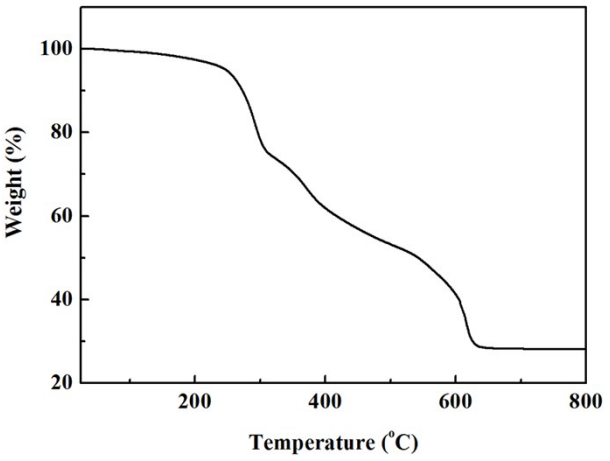


**Fig. S8** The TG curve of compound **1**.

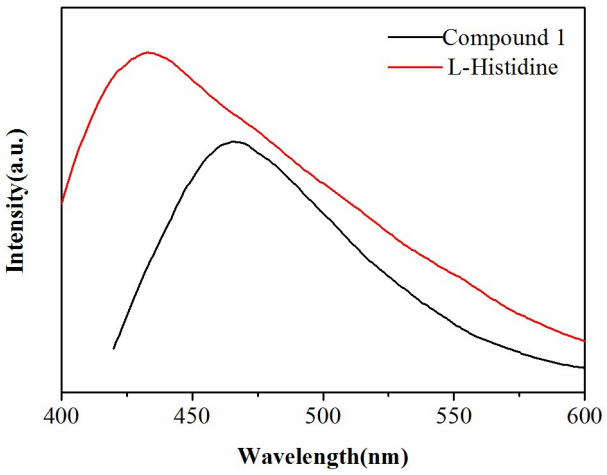


**Fig. S9** Room-temperature emission spectra of L-histidine and compound **1** (λex = 407 nm).

**Table S1**. Selected bond lengths [Å] and angles [deg.] for compound **1**.

| | | | |
|---|---|---|---|
| Zn1-O1 | 1.9247(18) | Zn1-O2[a] | 1.973(2) |
| Zn1-O4 | 1.9853(19) | Zn1-N1 | 1.989(2) |
| S1-O1 | 1.5362(19) | S1-O2 | 1.527(2) |
| S1-O3 | 1.5167(18) | | |
| O1-Zn1-O4 | 112.68(8) | O1-Zn1-O2[a] | 111.21(9) |
| O1-Zn1-N1[b] | 115.53(8) | O2[a]-Zn1-O4 | 102.49(8) |
| O4-Zn1-N1[b] | 107.54(8) | O2[a]-Zn1-N1[b] | 106.40(8) |
| O1-S1-O2 | 105.12(12) | O1-S1-O3 | 102.87(10) |
| O2-S1-O3 | 106.49(11) | Zn1-O1-S1 | 132.57(11) |
| Zn1[a]-O2-S1 | 125.46(12) | Zn1-C1-O4 | 117.34(17) |
| C4-N1-C6 | 105.9(2) | Zn1[c]-N1-C4 | 129.32(17) |
| Zn1[c]-N1-C6 | 123.62(19) | | |

Symmetry transformations used to generate equivalent atoms: [a] 1-x, 1-y, 1-z; [b] 3/2-x, -1/2+y, 3/2-z; [c] 3/2-x, 1/2+y, 3/2-z.

**Table S2** Hydrogen bonds for compound **1** [Å and deg.].

| D-H…A | d(D-H) | d(H…A) | D(D…A) | <DHA |
|---|---|---|---|---|
| O1W-H1W···O5 | 0.85 | 2.13 | 2.828(2) | 138.0 |
| N2-H2A···O5 | 0.89 | 1.97 | 2.848(3) | 168.0 |
| N2-H2B···O3 | 0.89 | 1.92 | 2.770(3) | 159.0 |
| N2-H2C···O3 | 0.89 | 2.06 | 2.877(3) | 152.0 |
| N3-H3···O3 | 0.86 | 1.94 | 2.791(3) | 168.0 |
| C2-H2···O4 | 0.98 | 2.55 | 3.288(3) | 132.00 |
| C5-H5…O5 | 0.93 | 2.54 | 3.100(3) | 119.0 |
| C6-H6···O2 | 0.93 | 2.60 | 3.426(3) | 149.0 |