Leakage and Proton Conductivity in the Predicted Ferroelectric $CsBiNb_2O_7$

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Supplementary material

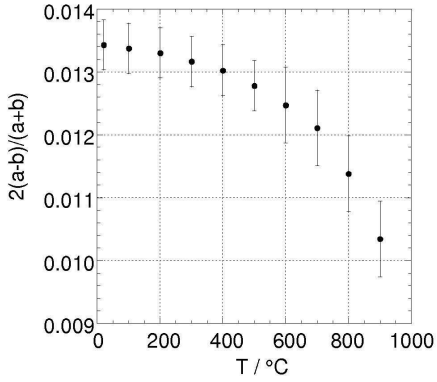

Figure S1. Orthorhombic distortion versus temperature for $CsBiNb_2O_7$

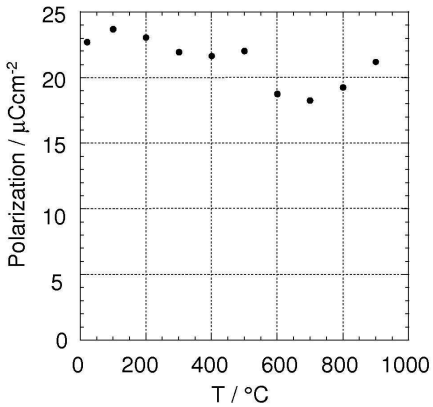

Figure S2. Calculated total ionic polarisation versus temperature for $CsBiNb_2O_7$

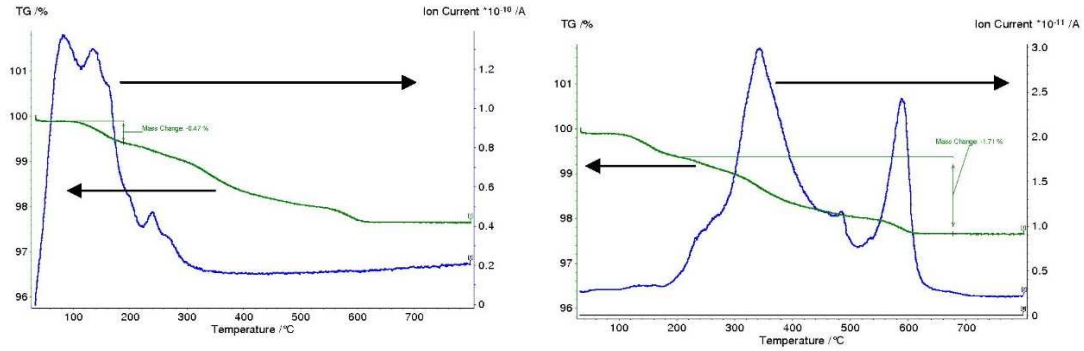

Figure S3. TGA-MS spectra for 'wet' $CsBiNb_2O_7$. (a) H_2O loss (b) CO_2 loss.

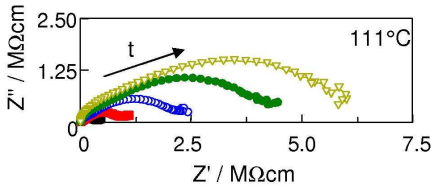

Figure S4. Z* plot as a function of time for data obtained at 111 °C in dry flowing N_2.

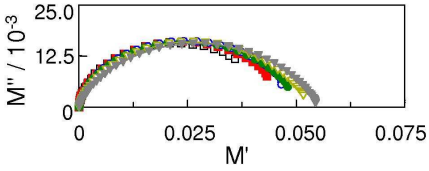

Figure S5. M* plots for data obtained in dry flowing N_2 at 155 (▼), 206 (▽), 260 (●), 291 (○), 326 (■) and 384 (□) °C.

The effect of changing the N_2 flow from dry to wet is shown in the form of combined spectroscopic Z″, M″ plots (Figure S6). The decrease in magnitude of Z″ shows the dramatic decrease in R_T and R_{gb} caused by the introduction of ionic conductivity. The height of bulk M″ peak remains constant indicating that C_b remains unchanged but the displacement of the peak to higher frequency with time indicates that the bulk conductivity is also increasing as moisture is introduced.

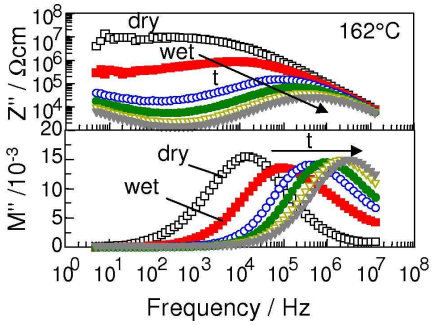

Figure S6. Spectroscopic Z′′,M′′ plots for data collected at 162 °C in dry N_2 (□) and as a function of time in N_2 passed through steam. Time intervals are *ca.* 10 mins. (Note logarithmic scale of Z′′ data.)

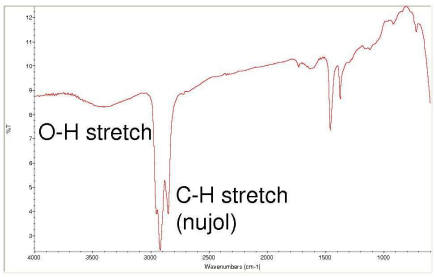

Figure S7. Typical IR spectrum for $CsBiNb_2O_7$ at 25 °C, exposed to air.