

--- Supporting Information ---

High-Resolution of Structural Water by ^{17}O NMR Spectroscopy

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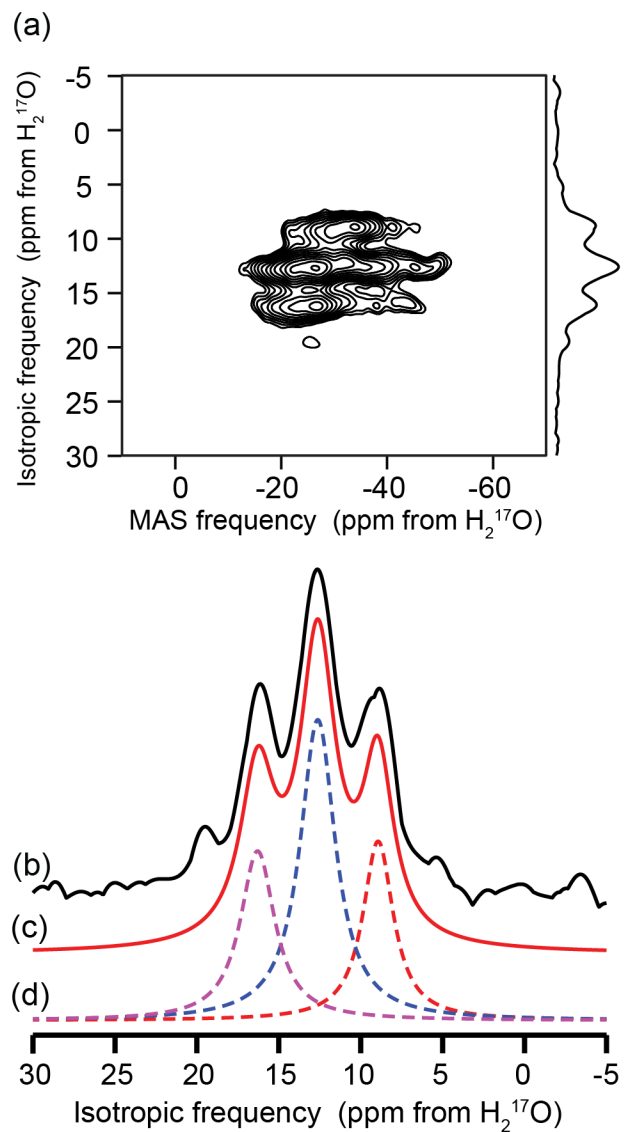


Figure S1: Experimental (a) ¹⁷O 2D MQMAS spectrum, and experimental (b) and fit (c,d) isotropic projections of the ¹⁷O 2D MQMAS spectrum at 21.1 T ($\omega_{\text{OH}}/2\pi = 900$ MHz). Three distinct water environments are resolved with isotropic frequencies of 8.9 ± 1 , 12.6 ± 1 , and 16.3 ± 1 ppm. The Gaussian fits of each environment (c,d) indicate a ratio of populations of 1:2:1.

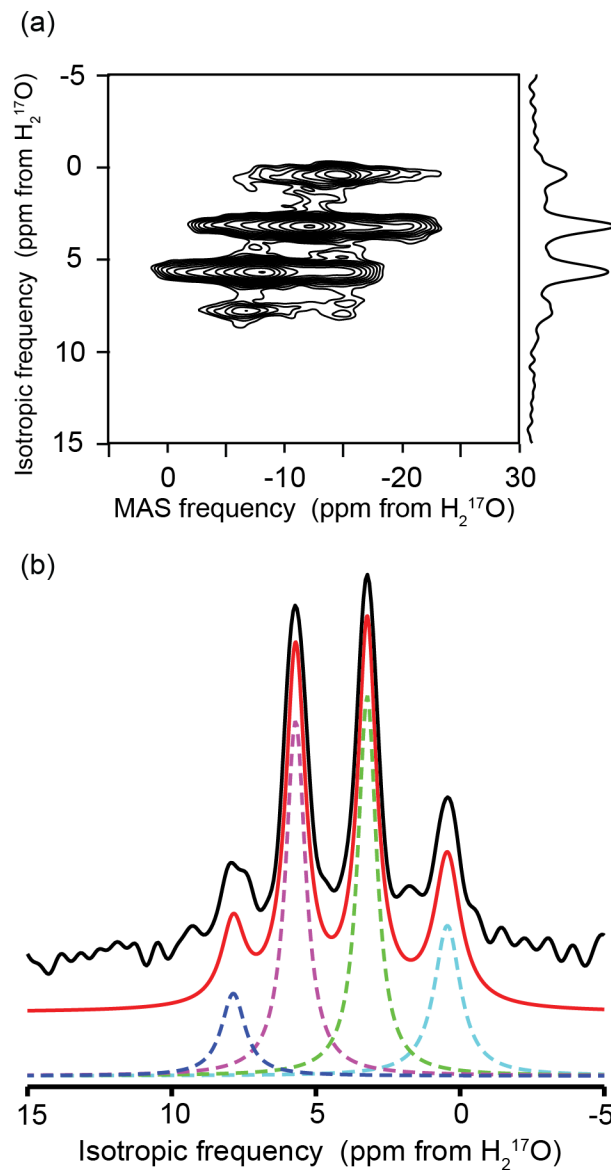


Figure S2: Experimental (a) ^{17}O 2D MQMAS spectrum, and experimental (b) and fit (c,d) isotropic projections of the ^{17}O 2D MQMAS spectrum at 35.2 T ($\omega_{\text{OH}}/2\pi = 1500$ MHz). Four distinct water environments are resolved with isotropic frequencies of 0.7 ± 1 , 3.4 ± 1 , 5.9 ± 1 , and 8.1 ± 1 ppm.

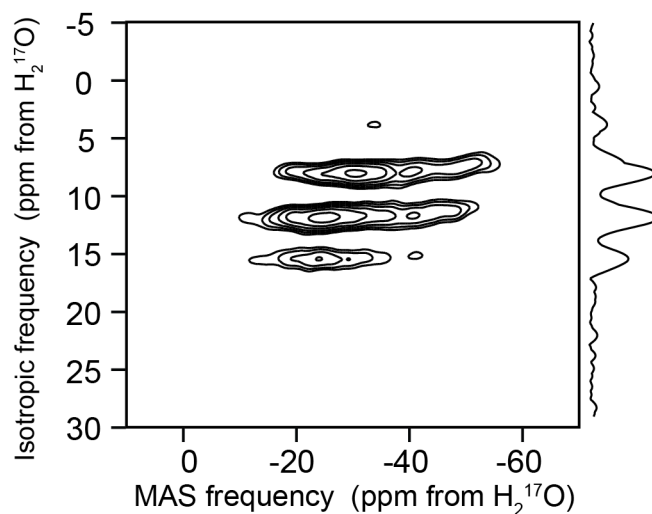


Figure S3: Oxygen-17 2D MQMAS NMR spectrum at 21.1 T ($\omega_{\text{OH}}/2\pi = 900$ MHz) with $\gamma B_1/2\pi = 100$ kHz continuous-wave ^1H decoupling. Three distinct water environments are resolved.

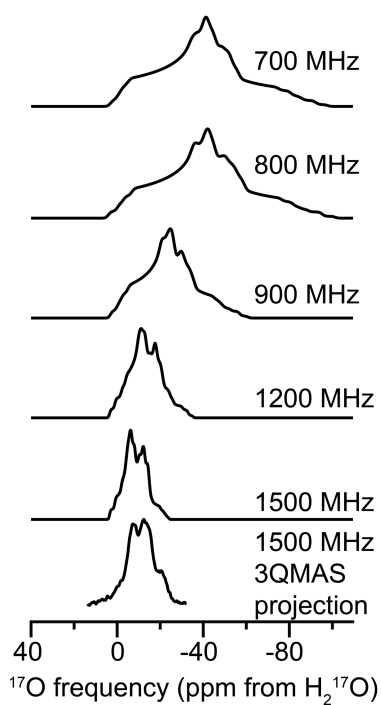


Figure S4: Simulated ^{17}O MAS NMR spectra at 16.4 to 35.2 T (700 to 1500 MHz, ^1H) and the projection of the direct 3QMAS dimension.