

The Structure and Activation of Substrate Water Molecules in Sr²⁺-Substituted
Photosystem II.†

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Supplementary Information

TITLE RUNNING HEAD: Two-Dimensional ^1H HYSCORE Spectroscopy of the S_2 State of Photosystem II.

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FIGURE CAPTIONS.

Figure 1S. The complete 2D HYSCORE spectrum of the (A) S_1 state and (B) S_2 of the OEC of Sr^{2+} -substituted PSII from *T. vulcanus* in protonated buffer at a magnetic field position of $g = 1.95$ with a τ delay of 140 ns.

Figure 2S. The skyline projection plot of the 2D HYSCORE spectrum of the S_1 state (red) and S_2 state (blue) of the OEC of Sr^{2+} -substituted PSII from *T. vulcanus* in protonated buffer with a τ delay of 140 ns.

Figure 3S. The frequency-squared representation of the 2D 1H HYSCORE spectrum of the OEC of Sr^{2+} -substituted PSII in protonated buffer at a magnetic field position of $g = 1.95$ with a τ delay of 140 ns.

Figure 4S. The 2D 1H HYSCORE difference spectrum of Ca^{2+} -containing and Sr^{2+} -substituted PSII from *T.vulcanus* in protonated buffer at a magnetic field position of $g = 1.95$ with a τ delay of 140 ns.

Figure 5S. The frequency-squared representation of the 2D 1H HYSCORE difference spectrum of Ca^{2+} -containing and Sr^{2+} -substituted PSII from *T.vulcanus* in protonated buffer at a magnetic field position of $g = 1.95$ with a τ delay of 140 ns. The dotted lines represent the diagonal and the least square linear fit of the proton hyperfine ridges W^I and W^{II} .

Figure 1S.

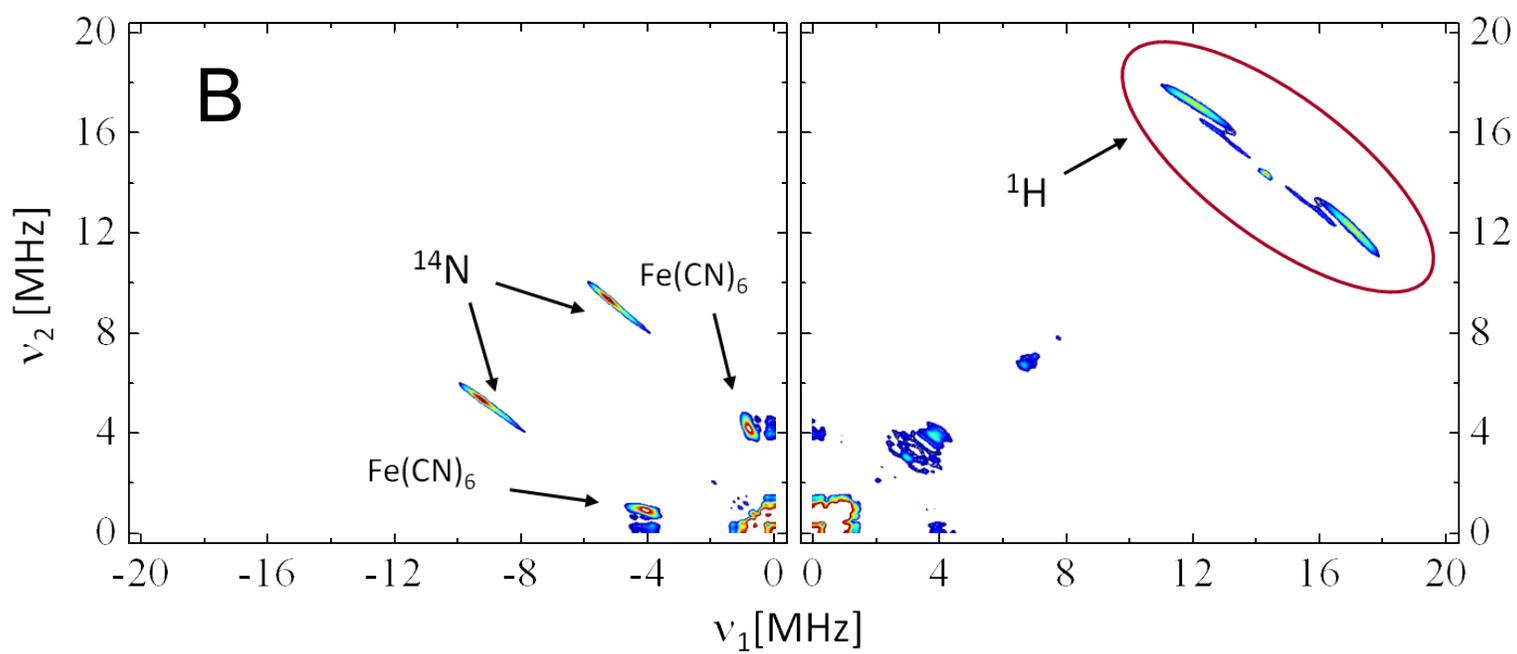
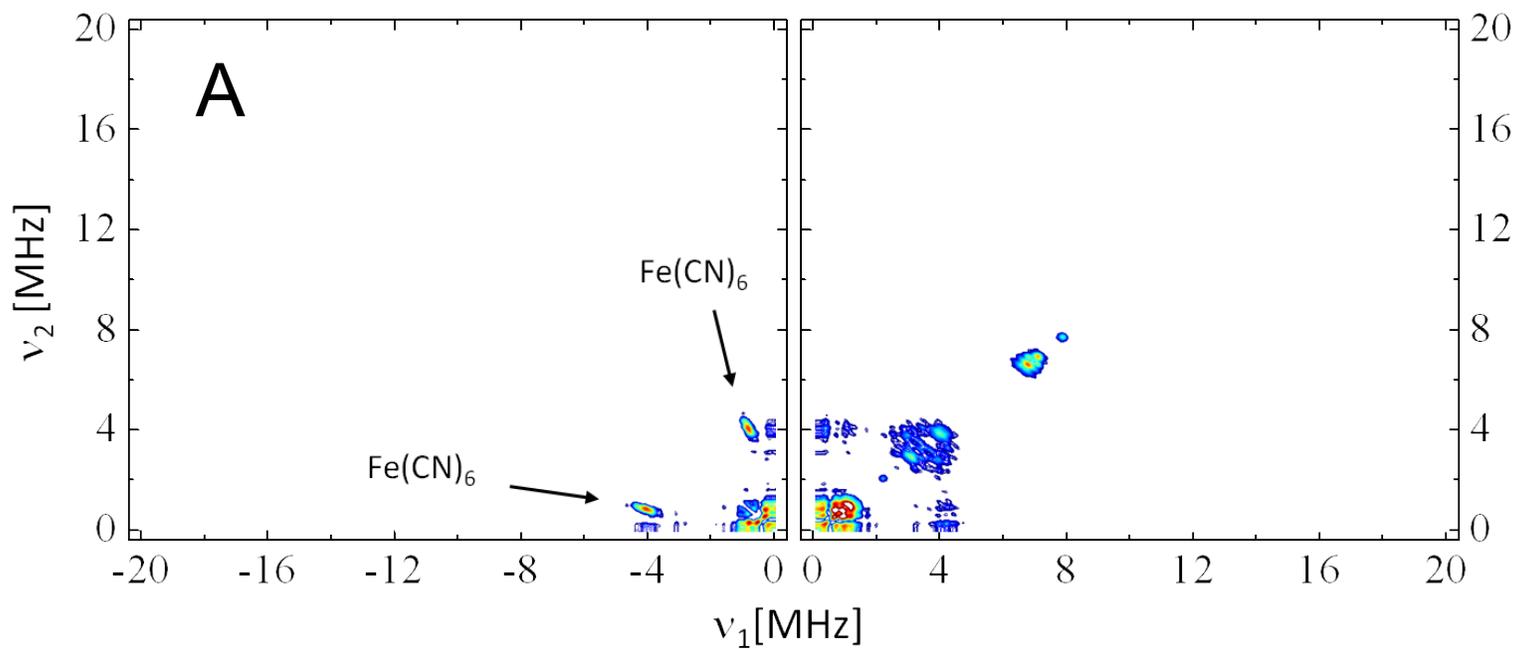


Figure 2S.

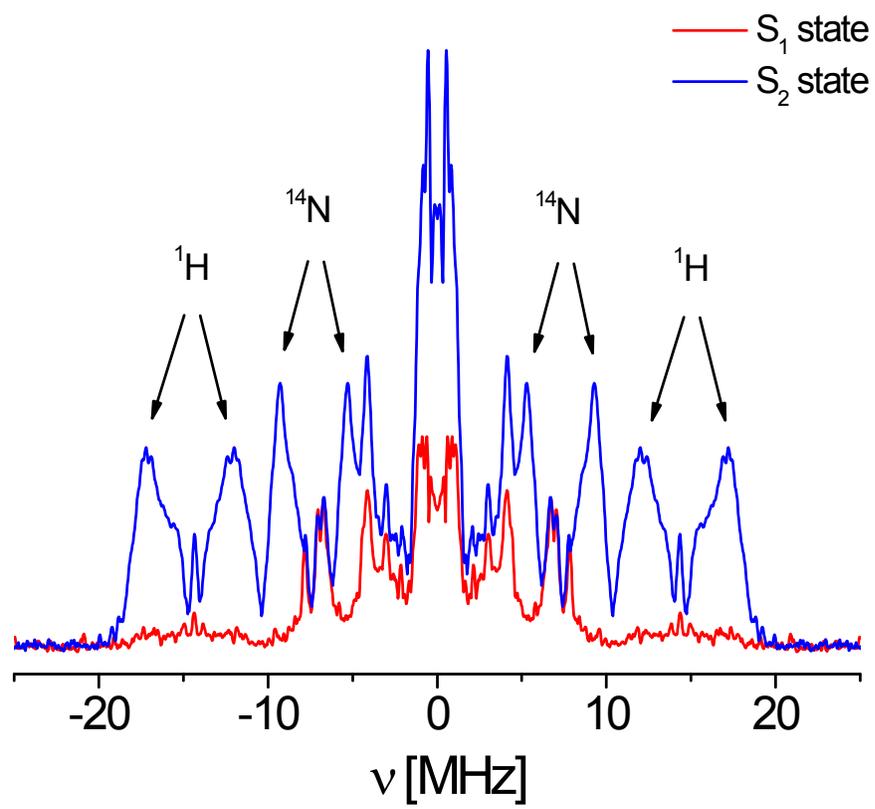


Figure 3S.

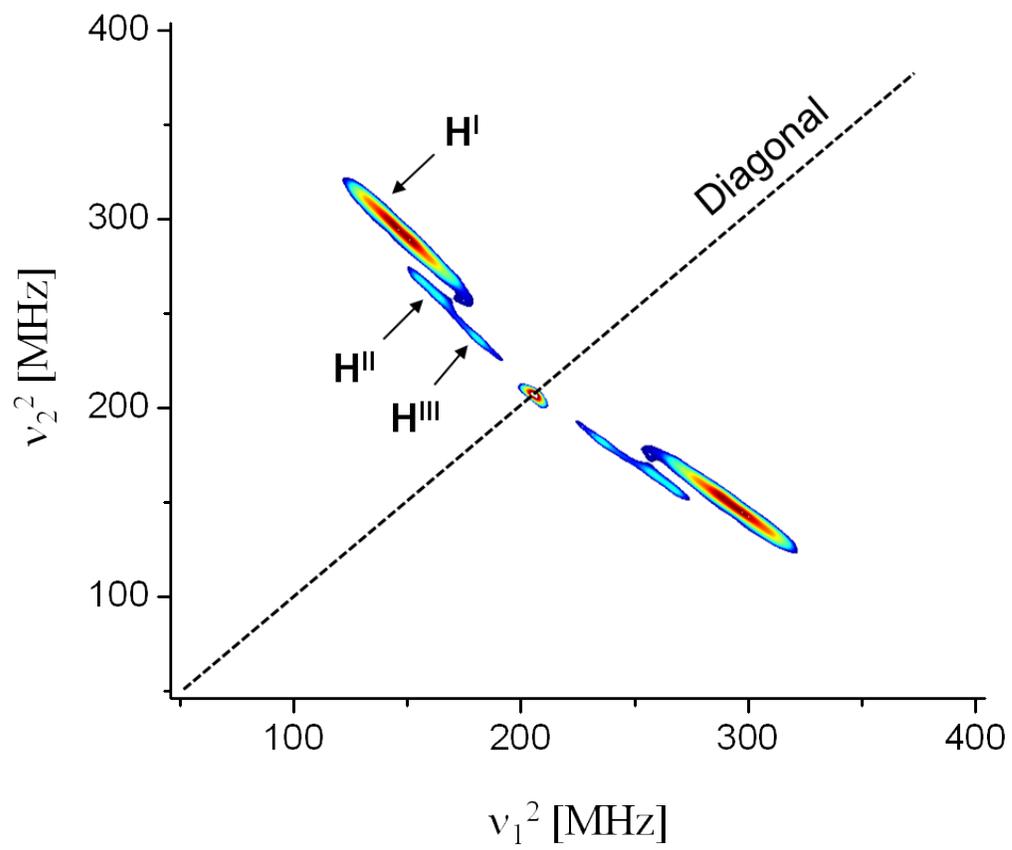


Figure 4S.

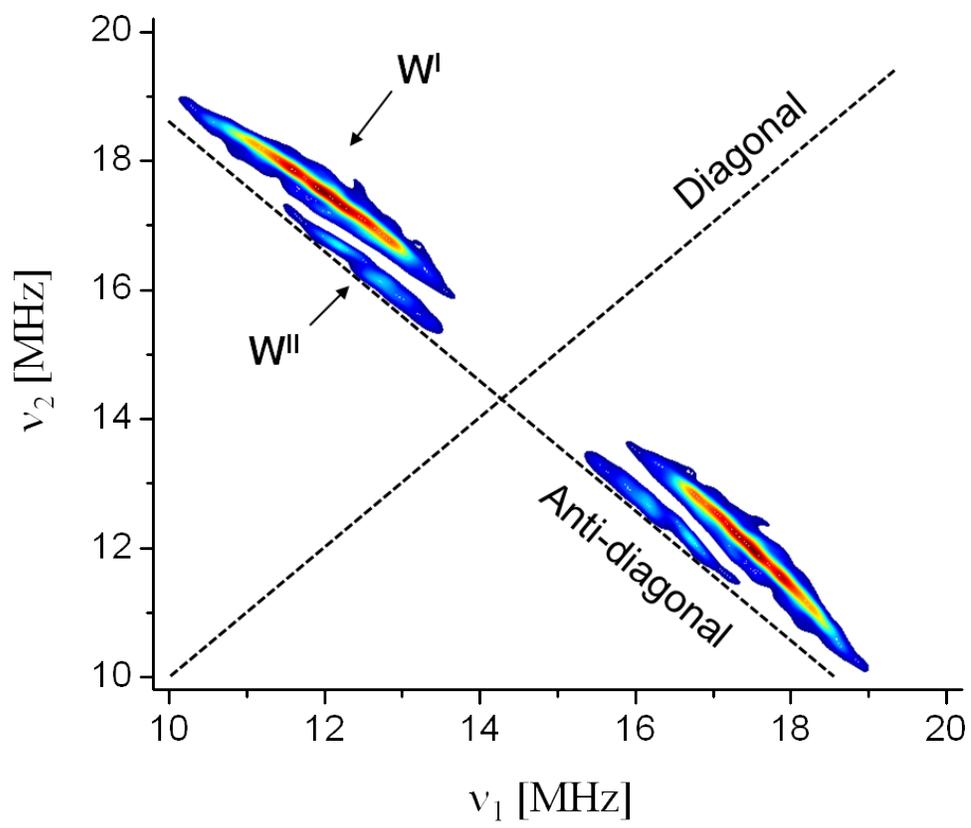


Figure 5S.

