Supporting Information

Energetics of the S_2 State Spin Isomers of the Oxygen-Evolving Complex of Photosystem II

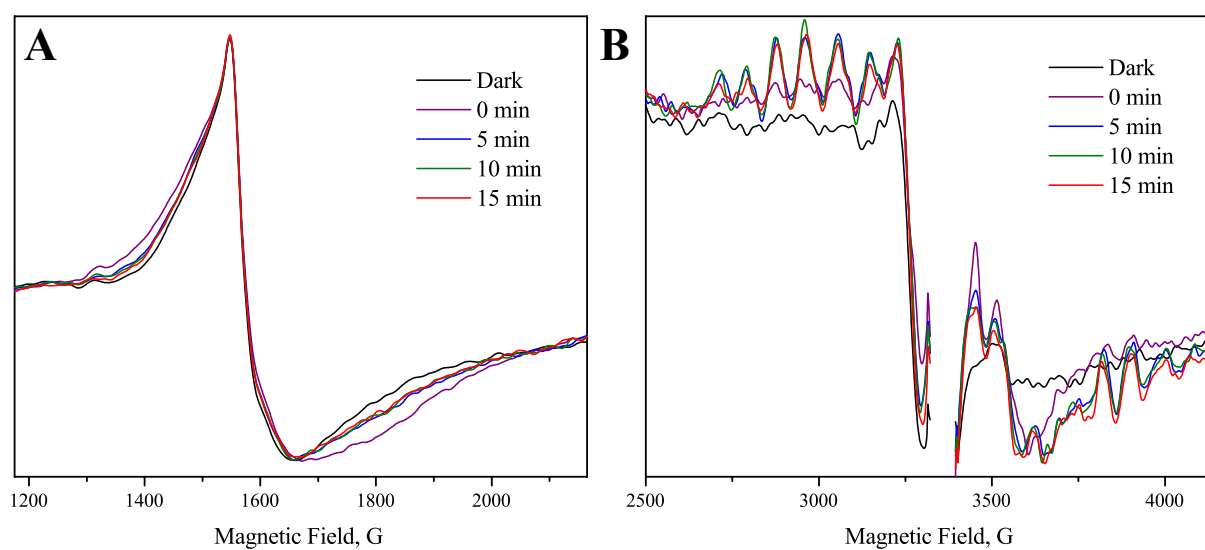David J. Vinyard, Sahr Khan, Mikhail Askerka, Victor S. Batista and Gary W. Brudvig

Figure S1. Unsubtracted EPR spectra from Figure 2A highlighting the $g = 4.1$ (A) and $g = 2$ (B) signals.
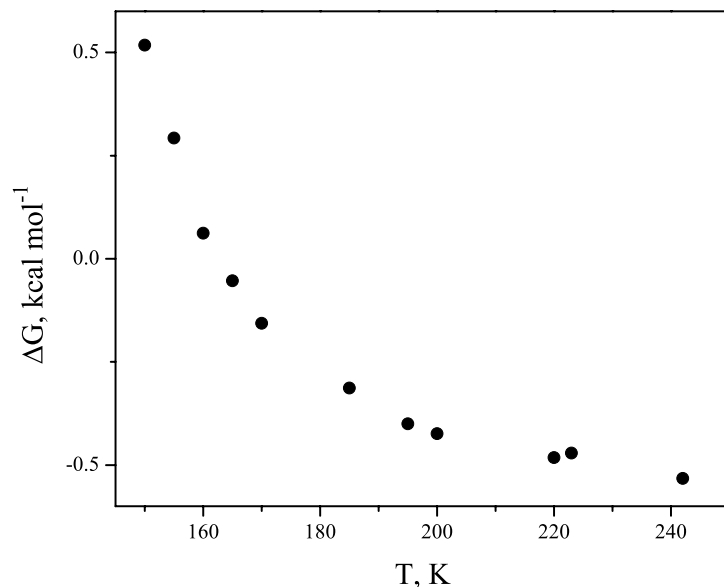
Figure S2. Temperature dependence of the free energy of conversion of the S_2 state $S = 5/2$ spin isomer to the S_2 state $S = 1/2$ spin isomer.
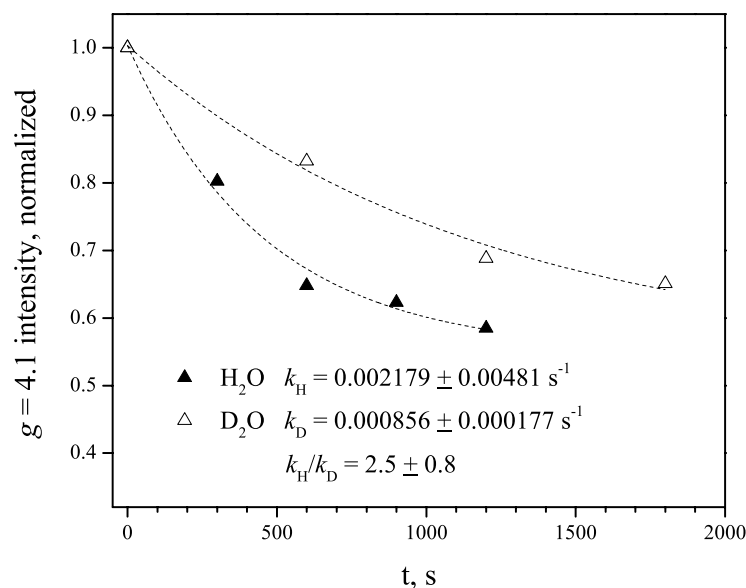Data from Figure 3 were re-plotted where $\Delta G = -RT \ln K$.

Figure S3. H/D kinetic isotope effect of conversion of the S_2 state $S = 5/2$ isomer to the S_2 state $S = 1/2$ isomer at 160 K. H_2O data (closed triangles) are identical to those shown in Figure S1. D_2O data (open triangles) were collected on a sample prepared as described above but in 99% D_2O at pD 6.0. Data were fit to a single exponential decay ($y = y_0 + A*\exp(-x/t)$).
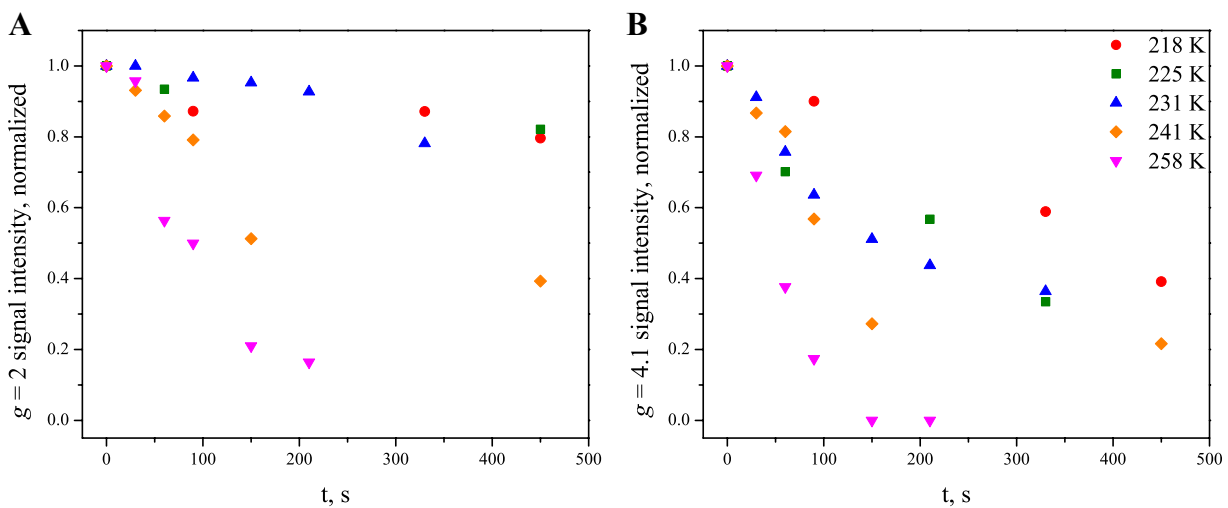
Figure S4. Kinetics of decay of the $S = 5/2$ spin isomer and the $S = 1/2$ spin isomer. Normalized peak-to-peak heights of the $g = 2$ (A) and $g = 4.1$ (B) EPR signals vs. incubation time.
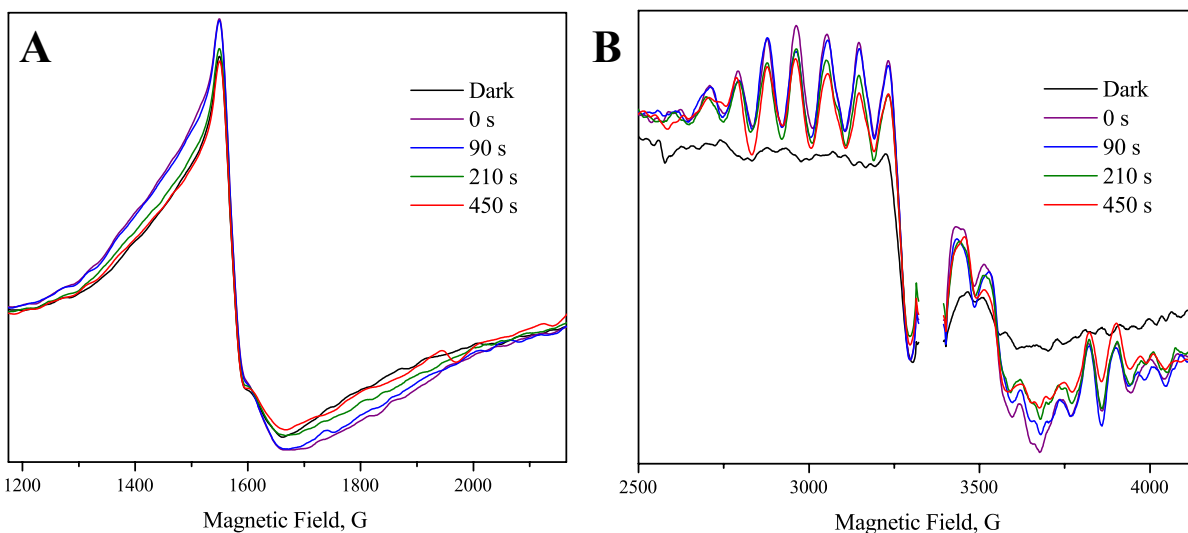

Figure S5. Unsubtracted EPR spectra from Figure 5A highlighting the $g = 4.1$ (A) and $g = 2$ (B) signals.