Electronic Supporting Information

Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S₂ state: a combined EPR and DFT study

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S1 PSII sample preparation

In native and Sr^{2+} substituted samples, the S₂ state was generated by short white-light illumination (5 s) with a tungsten lamp at 200 K, , using an ethanol bath cooled with dry ice.

Ammonia was added to the samples as follows. A stock solution of 1 M ammonium chloride (¹⁴NH₄Cl) in 1 M HEPES buffer set to a pH of 7.5 was made. For Q- and W-band samples, this solution was then added to the photosystem II (PSII) sample at a ratio of 1:10 (v/v), yielding a concentration of the free base NH₃ of 2 mM. The samples were reconcentrated using Millipore microcentrifuge filters to the desired concentration. Afterwards, the sample was placed in a Q- or W-band tube, left in complete darkness for ≈ 10 min and frozen for experiments in the S₁ state. To generate the NH₃-modified S₂ state, the sample was first illuminated at 200 K for 5 s and then subsequently annealed at \approx 260 K (ethanol/dry ice) for 20-30 s before freezing to 77 K (liquid N₂). A similar procedure was used for X-band samples. Here though, the PSII sample was placed in the X-band tube and given two saturating light flashes prior to the addition of ¹⁴NH₄Cl solution. There was a one-hour delay between the two light flashes and the addition of NH₃, during which the sample was kept in complete darkness. Phenyl-p-benzoquinone (PPBQ) dissolved in dimethyl sulfoxide (DMSO) was added to the sample immediately prior to the addition of ¹⁴NH₄Cl solution. After incubation for 2-3 min, the sample was frozen to first record spectra in the dark-adapted state. Subsequent illumination at 180 K (ethanol/liquid N₂) followed by an annealing step at 0 °C (ice/water) for 10-20 s generated the NH₃-modified S₂ state.

S2 Data processing: baseline correction and light-minus-dark subtraction

To minimize possible contributions from underlying signals from other paramagnetic species in the sample, such as hexaquo-Mn^{II}, oxidized cytochrome b_{559} and c_{550} and Fe^{II}/Q_A⁻, S₂-minus-S₁ (light-minus-dark) subtractions were performed for X- and Q-band pulse EPR and electron nuclear double resonance (ENDOR) spectra. From derivative-shaped, *i.e.* continuous wave (CW) or pseudo-modulated, EPR spectra a fitted baseline was subtracted.

Three-pulse electron spin echo envelope modulation (ESEEM) data were also baseline-corrected after light-minus-dark subtraction of the normalized time-domain traces. (Fig. S1), in order to obtain spectra containing only resonances from the oxygen-evolving complex (OEC) in the S₂ state, excluding modulations from other paramagnetic species, foremost the background cytochrome (¹⁴N) signals. The (T_1) decay was modeled and removed by subtracting a third (X-band), a fifth (Q-band Mn₄O₅Ca, Mn₄O₅Sr) or seventh (Q-band Mn₄O₅Ca–NH₃) order polynomial fit function from the light-minus-dark difference.

Hyperfine sublevel correlation (HYSCORE)-spectroscopic data were baseline corrected using polynomial fit curves in both dimensions. Before Fourier transformation, a hamming apodization window and zero-filling were applied to the individual ESEEM and HYSCORE spectra. Experimental and simulated X-band ESEEM spectra were normalized with respect to the time domain spectra. Frequency-domain HYSCORE spectra and simulations were normalized with respect to the height of the single-quantum ¹⁴N peaks.

Electron electron double resonance (ELDOR)-detected NMR (EDNMR) spectra were baselinesubtracted and further processed to obtain an ENDOR-like representation of the spectra as described in Ref.¹.

S4



Fig. S1 Example for the light-minus-dark subtraction and baseline correction of three-pulse ESEEM spectra. The solid black and red lines depict ESEEM spectra of a PS II sample in the S₂ (1) and S₁ states (2), after subtraction of the y-axis offset and normalization. The blue solid line shows the spectrum resulting from the S₂-minus-S₁ subtraction (3). The superimposing green dashed line (4) represents a fifth order polynomial fit curves to (3). The solid orange line (5) is the baseline-corrected resulting ESEEM spectrum after background subtraction. Experimental parameters: magnetic field: 1220 mT, τ : 260 ns; other settings were those given in Fig. S4.

The EasySpin^{2, 3} function 'pepper' was used to calculate EPR spectra, 'salt' for ENDOR, 'saffron' for three-pulse ESEEM and HYSCORE and a home-written script involving EasySpin functions for EDNMR spectra.

For calculation of the spin Hamiltonians of the ⁵⁵Mn tetramer-single electron spin manifolds that describe the EPR and ⁵⁵Mn-ENDOR spectra, the electron Zeeman term was treated exactly. The ⁵⁵Mn hyperfine terms were treated using second order perturbation theory. ⁵⁵Mn nuclear quadrupole interactions (NQI) are not resolved in both the EPR and ENDOR spectra and thus omitted in their simulations. The ⁵⁵Mn nuclear Zeeman terms were not included in the EPR simulations (see sections S4.2 and S4.3). The *G* and the four effective ⁵⁵Mn hyperfine tensors A_i were assumed to be collinear. First-derivative X- and Q-band EPR, and absorption-line W-band EPR and Q-band ⁵⁵Mn-ENDOR data were simultaneously fit using a least squares routine.

For simulation of the (orientation-selective) ESEEM, HYSCORE and EDNMR spectra, ¹⁴N, ¹⁵N and ¹⁷O single nucleus-single electron spin Hamiltonians were used. The ⁵⁵Mn nuclear interactions were not considered explicitly, but accounted for by employing hyperfine strain, *i.e.* an isotropic broadening due to unresolved hyperfine couplings, to compute the excitation window. All other spin Hamiltonian terms were treated exactly. In the simulations of the ¹⁷O-EDNMR spectra, the NQI term was omitted as it is not resolved within the line width.

ESEEM simulation traces were fitted to the time-domain spectra. The X-band ESEEM spectra were fitted including two nitrogen nuclei and contributions from ¹H nuclei simulated by a hyperfine interaction $A_i = [-0.44 - 0.44 + 1.44]$ MHz.

EDNMR transition intensities were calculated assuming small angle excitation by the high turning angle (HTA) pulse, as described in Cox *et al.* ⁴. As in Refs. ^{1, 5}, the contributions from different nuclear species, as well as their individual single- and double-quantum transition envelopes, were calculated and normalized separately. Specifically, for the ¹⁷O signal envelopes, which are made up of multiple species,

the fitting was constrained such that the relative intensities of the different contributions were scaled according to the magnitude of the anisotropic component of the hyperfine interaction.

S4 Theoretical background

S4.1 The spin Hamiltonian formalism. Here, we consider a single ligand ¹⁴N, ¹⁵N or ¹⁷O nucleus magnetically interacting with an exchange-coupled Mn tetramer. The current assignment for the oxidation states of the four Mn ions when poised in the S₂ state is $Mn^{III}Mn^{IV}Mn^{IV}Mn^{IV}$.⁶⁻¹³ This net oxidation state is assumed throughout the text. A basis set that describes the ¹⁴N-, ¹⁵N- or ¹⁷O-Mn-tetramer spin manifold can be built from the product of the eigenstates of the interacting spins:

$$|S_1S_2S_3S_4M_1M_2M_3M_4I_1I_2I_3I_4m_1m_2m_3m_4Lk\rangle,$$
(Eq. S1)

Here, S_i (with i = 1 - 4) refers to the electronic spin state of Mn_i, M_i refers to the electronic magnetic sublevel of Mn_i, I_i refers to the nuclear spin state of Mn_i, and m_i refers to the nuclear magnetic sublevels of Mn_i. S_i takes the value 2 for Mn^{III} and 3/2 for Mn^{IV}; M_i takes the values: S_i , S_i -1,, 1- S_i , $-S_i$; I_i takes the value 5/2 for ⁵⁵Mn, m_i takes the values $-I_i$, 1- I_i ,, I_i -1, I_i , L takes the values 1 for ¹⁴N, ¹/₂ for ¹⁵N and 5/2 for ¹⁷O, and k takes the values -L, 1-L,, L-1, L.

The spin Hamiltonian that describes the spin manifold of the ¹⁴N-, ¹⁵N- or ¹⁷O-Mn tetramer is:

$$H = \sum_{i} \beta_{e} \vec{B}_{0} \cdot \hat{g}_{i} \cdot \vec{S}_{i} + \sum_{i} \vec{S}_{i} \cdot \hat{d}_{i} \cdot \vec{S}_{i} + \sum_{i < j} \vec{S}_{i} \cdot \hat{J}_{ij} \cdot \vec{S}_{j} - \sum_{i} g_{Mn} \beta_{n} \vec{B}_{0} \cdot \vec{I}_{i} + \sum_{i} \vec{S}_{i} \cdot \hat{a}_{Mn,i} \cdot \vec{I}_{i}$$
$$+ \sum_{i} \vec{I}_{i} \cdot \hat{q}_{Mn,i} \cdot \vec{I}_{i} - g_{L} \beta_{n} \vec{B}_{0} \cdot \vec{L} + \vec{S}_{L} \cdot \hat{a}_{L} \cdot \vec{L} + \vec{L} \cdot q_{L} \cdot \vec{L}$$
(Eq. S2)

It contains (i) an electronic Zeeman term for each Mn (g_i) ion, (ii) a fine structure term for each Mn (d_i) ion, and (iii) pair-wise electronic exchange terms for each Mn-Mn (J_{ij}) interaction, (iv) a nuclear Zeeman term for each ⁵⁵Mn (g_{Mn}) nucleus and the ligand (g_L) nucleus, (v) an electron-nuclear hyperfine term for each ⁵⁵Mn ($a_{Mn,i}$) nucleus and the ligand (a_L) nucleus (vi) an NQI term for each ⁵⁵Mn ($q_{Mn,i}$) and the ligand (q_L) nucleus.

S4.2 An effective spin $S_T = \frac{1}{2}$ ground state. A basis set that describes the entire spin manifold of the coupled four ⁵⁵Mn ions of the OEC requires 414720 vectors, too many to be readily handled by current numerical techniques. The problem can be greatly simplified by assuming that all Mn-Mn couplings are large, *i.e.* within the strong exchange limit. For this to apply, the exchange interactions between the Mn ions have to be significantly larger than any other term of the spin Hamiltonian. The resultant electronic spin states of the manifold are then adequately described by a single quantum number, the total spin (S_T) . The multiline EPR signal observed for the S₂ state of the OEC is derived from only one total spin state, the ground state of the spin manifold with total spin $S_T = \frac{1}{2}$. The basis set that describes this subspace requires only 15552 vectors in the case that models the coupling of the effective electronic spin $(S_T = \frac{1}{2})$ to the nuclear spin of each ⁵⁵Mn ($I = \frac{5}{2}$) and a single ligand (L) nucleus:

$$\begin{vmatrix} \frac{1}{2} & M & I_1 & I_2 & I_3 & I_4 & m_1 & m_2 & m_3 & m_4 & L & k \end{vmatrix}$$
 (Eq. S3)

Where *M* takes all half-integer values $-\frac{1}{2} \le M \le \frac{1}{2}$, m_i takes all half-integer values $-\frac{5}{2} \le m_i \le \frac{5}{2}$, and *k* takes values $-L \le k \le L$.

The effective spin Hamiltonian that describes the ground state of the spin manifold ($S_T = \frac{1}{2}$) is:

$$H = \beta_{\rm e}\vec{B}_0 \cdot \hat{G} \cdot \vec{S} + \sum_i \left(-g_{\rm Mn}\beta_{\rm n}\vec{B}_0 \cdot \vec{I}_i + \vec{S} \cdot \hat{A}_{{\rm Mn},i} \cdot \vec{I}_i \right) - g_{\rm L}\beta_{\rm n}\vec{B}_0 \cdot \vec{L} + \vec{S}_L \cdot \hat{A}_L \cdot \vec{L} + \vec{L} \cdot q_{\rm L} \cdot \vec{L} \quad (\text{Eq. S4})$$

It contains, (i) the Zeeman term for the total electronic spin, (ii) Zeeman terms for each ⁵⁵Mn and the ligand nucleus, (iii) hyperfine terms for each ⁵⁵Mn and the ligand nucleus and (iv) a quadrupole term for the ligand nucleus. Quadrupole terms are neglected for the ⁵⁵Mn nuclei as their size is smaller than the fitted line width.

S4.3 Application to the different spectroscopic experiments. The simulation of spectra from EPR and related experiments probing electronic spin transitions of the OEC can be further simplified. As the ligand couplings are comparatively small, they do not significantly contribute to the inhomogeneous line width of the S_2 state EPR spectrum. Thus, for simulation of the EPR spectrum, the terms in Eq. S4 relating to the ligand nucleus can be excluded (Eq. S5).

$$H_{\rm EPR} = \beta_{\rm e} \vec{B}_0 \cdot \hat{G} \cdot \vec{S} + \sum_i \vec{S} \cdot \hat{A}_{{\rm Mn},i} \cdot \vec{I}_i$$
(Eq. S5)

Also, a simplified effective spin Hamiltonian can be used for the simulation of the spectra from experiments probing nuclear magnetic interactions, as the various nuclei do not significantly couple to each other. Thus, for the simulation of the ⁵⁵Mn-ENDOR resonances, terms in Eq. 4 associated with the ligand nucleus can be excluded:

$$H_{\rm MnENDOR} = \beta_{\rm e} \vec{B}_0 \cdot \hat{G} \cdot \vec{S} + \sum_i \left(-g_{\rm Mn} \beta_{\rm n} \vec{B}_0 \cdot \vec{I}_i + \vec{S} \cdot \hat{A}_{{\rm Mn},i} \cdot \vec{I}_i \right)$$
(Eq. S6)

Similarly, for describing the nuclear interactions of a ligand ¹⁴N, ¹⁵N or ¹⁷O nucleus in the various experiments (ESEEM, HYSCORE, EDNMR), the terms relating to the ⁵⁵Mn nuclei in Eq. 4 can be omitted:

$$H_{\text{Ligand}} = \beta_{\text{e}} \vec{B}_0 \cdot \vec{G} \cdot \vec{S} - g_{\text{L}} \beta_{\text{n}} \vec{B}_0 \cdot \vec{L} + \vec{S}_{\text{L}} \cdot \hat{A}_{\text{L}} \cdot \vec{L} + \vec{L} \cdot q_{\text{L}} \cdot \vec{L}$$
(Eq. S7)

In practice, however, the spin Hamiltonian in Eq. S7 is only valid when an ESEEM, ENDOR or EDNMR spectrum is collected at the center field of the S_2 state multiline spectrum as at this position all powder pattern orientations are sampled uniformly. Especially at W-band, spectra collected on the high-and low-field edges of the multiline spectrum must also take into account the sampling of the powder pattern orientations, which for the S_2 state ⁵⁵Mn tetramer is defined by the hyperfine coupling of the ⁵⁵Mn nuclei along with the *G* tensor. Eq. S7 can still be used (*i.e.*, terms associated with the ⁵⁵Mn nuclei can be excluded), but each orientation must include a weighting derived from simulation of the EPR line shape, for which the ⁵⁵Mn hyperfine interactions are taken account by hyperfine strain.

S5

DFT calculations: NH₃ binding modes and spatial coordinates of the S₂ state models



Fig. S2 Optimized structures (only the inorganic core framework and the terminal Mn_{A4} ligands are shown) and relative energies in kcal/mol of alternative models for NH₃, NH₂ and NH binding. The five structures on the left and the two structures on the right form two isomer sets. Although the complexity of the OEC structure and the extensive hydrogen bonding between terminal ligands and the surrounding residues and H₂O molecules make it difficult to isolate the structural origin of all energy differences, the results demonstrate unambiguously that terminal NH₃ coordination by W1 displacement (top left) is the energetically preferred interaction mode of ammonia with the OEC cluster.

S5.2 Cartesian coordinates of the optimized DFT structures

Mn₄O₅Ca

Mn	-24.848563	-35.523079	203.967881
Mn	-27 334886	-35 213752	205 224408
1	27 224054	22 247504	202 12000
1111	-27.324954	-33.34/594	203.139009
Mn	-27.586920	-33.190450	200.400671
Ca	-27 866960	-36 744419	202 214036
04	27.0000000	26 501015	202.211000
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0	-28.351166	-34.735051	203.786382
\cap	-26 000441	-34 050081	201 176135
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0	-26.773447	-34.313956	201.661037
\cap	-28 452549	-31 704459	199 310367
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0	-26.6/3182	-33.801897	198.9102/9
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U	-21.42/294	-30.009813	204.064009
С	-20.718700	-32.621528	201.484318
С	-21.588166	-33.370625	202.438984
C	-22 935559	-33 687611	202 415622
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С	-22.142018	-34.418977	204.333486
Ν	-23.257629	-34.340485	203.596833
N	-21 804706	-29 583301	202 173241
	21.001/00	20.015010	202.1/3241
C	-22.89630/	-28.815019	202./591/1
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$\begin{array}{c} + & -30.304360 & -30.649272 & 208.998603 \\ - & -30.997751 & -31.051074 & 208.236197 \\ + & -31.843803 & -31.521736 & 208.767318 \\ \hline & -29.032035 & -31.540173 & 206.658983 \\ \hline & -28.353578 & -32.561403 & 205.766910 \\ \hline & -28.097633 & -33.716666 & 206.279018 \\ \hline & -28.097633 & -33.716666 & 206.279018 \\ \hline & -28.097633 & -32.210782 & 204.577261 \\ + & -36.663406 & -31.800759 & 206.877175 \\ \hline & -36.971479 & -32.276075 & 205.926511 \\ \hline & -35.741686 & -32.750576 & 205.123250 \\ \hline & -35.741686 & -32.750576 & 205.123250 \\ \hline & -33.683948 & -34.348734 & 205.1636355 \\ \hline & -32.719724 & -33.611907 & 205.957189 \\ \hline & -33.683948 & -34.348734 & 205.1636355 \\ \hline & -31.757597 & -33.834930 & 203.664614 \\ \hline N & -31.543259 & -35.145308 & 203.457803 \\ \hline & -31.047224 & -32.940683 & 202.962512 \\ O & -27.559854 & -29.319219 & 204.115328 \\ H & -32.769260 & -42.810763 & 197.017851 \\ H & -33.346737 & -41.144690 & 197.229596 \\ H & -33.700323 & -42.030393 & 195.723193 \\ H & -31.728017 & -40.338448 & 195.460444 \\ H & -31.188644 & -42.007082 & 195.180287 \\ H & -30.190114 & -43.321384 & 197.193914 \\ H & -28.664658 & -43.179784 & 199.154699 \\ H & -27.525101 & -41.846717 & 200.701984 \\ H & -27.647817 & -37.542060 & 207.671113 \\ H & -28.778547 & -37.542060 & 207.671113 \\ H & -27.647817 & -37.542060 & 207.671113 \\ H & -27.647817 & -37.542060 & 207.671113 \\ H & -22.972246 & -45.417617 & 202.197588 \\ H & -23.899004 & -46.164471 & 199.969225 \\ H & -23.385908 & -44.631971 & 199.230247 \\ H & -22.524127 & -38.841811 & 201.510847 \\ H & -24.048025 & -40.767550 & 201.513805 \\ H & -23.385908 & -44.631971 & 199.230247 \\ H & -22.524127 & -38.841811 & 201.510847 \\ H & -24.306083 & -40.660102 & 203.264364 \\ H & -26.357875 & -29.742211 & 209.595398 \\ H & -23.687705 & -33.541102 & 201.616471 \\ H & -22.097321 & -34.868618 & 205.315170 \\ H & -19.696150 & -30.723618 & 201.264263 \\ \end{array}$	0	-20.81/100	-39.052364	203.09/592
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C -33.683948 -34.348734 205.163635 N -32.719724 -33.4348734 205.163635 N -31.757597 -33.834930 203.664614 N -31.047224 -32.940683 202.962512 O -27.559854 -29.319219 204.115328 H -32.769260 -42.810763 197.017851 H -33.346737 -41.144690 197.229596 H -33.700323 -42.030393 195.723193 H -31.728017 -40.338448 195.460444 H -31.188644 -42.007082 195.180287 H -30.190114 -43.321384 197.193914 H -28.664658 -39.019225 197.260996 H -29.160345 -38.882656 199.243123 H -30.698698 -39.019225 197.260996 H -27.647817 -37.542060 207.671113 H -27.647817 -37.533001 210.268672 H -21.67653 -43.090833	Ĉ	-34 772092	-33 611907	205 957189
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Fig. S3 Comparison of Q-band ⁵⁵Mn-ENDOR spectra of PSII samples isolated from *T. elongatus* in the native (Mn₄O₅Ca, black), Sr²⁺-substituted (Mn₄O₅Ca, red) and NH₃-annealed (Mn₄O₅Ca–NH₃, blue) S₂ states recorded without (top traces) and with (bottom traces)⁵ radio frequency (RF) matching employed. Shown are the spectra of illuminated samples without light-minus-dark subtraction. Experimental parameters: microwave frequencies: 33.9678 GHz (top, black), 33.9950 GHz (top, red), 34.0053 GHz (top, blue), 34.0368 GHz (bottom, black), 34.0435 GHz (bottom, red), 34.0159 GHz (bottom, blue); magnetic field: 1220 mT; shot repetition time: 1 ms; microwave pulse length (π): 32 ns (top), 24 ns (bottom); τ : 268 ns; RF pulse length (π_{RF}): 3.5 µs; temperature: 4.8 K (top), 5.2 K (bottom).

In order to overcome variations of the spectral shape, especially at higher frequencies (>150 MHz), the ⁵⁵Mn-ENDOR experiments presented here were performed under instrumental settings that allowed for the best reproducibility. To obtain cleaner spectra, a radio frequency (RF) matching network, usually employed for producing a more uniform, frequency-independent RF amplitude to suppress artifacts and distortions of the spectral baseline, was omitted. Our optimization of the experimental conditions rationalizes spectral differences from earlier published Q-band data^{5, 12, 13}, in which the higher frequency resonances (> \approx 140 MHz) were comparatively suppressed, their maxima appearing shifted to somewhat lower frequencies (Fig. S3).* This is reflected in the fitted hyperfine tensor components reproducing these spectra. While the magnitudes $A_{i,iso}$ of the four ⁵⁵Mn hyperfine tensors are approximately the same as those determined in PSII from higher plants and cyanobacteria,^{5, 9, 10, 12, 13} the size of the effective anisotropic components $A_{i,aniso}$ differ. This can be rationalized spectrally by the intensity profiles of the actual ⁵⁵Mn-ENDOR signals, specifically the relative enhancement of the two peaks at highest radio frequencies, yielding a more isotropic largest hyperfine tensor A_1 . This in turn requires the other three tensors A_2 , A_3 and A_4 to be less isotropic. Furthermore, reduced orientation selectivity, by employing harder, *i.e.* shorter microwave pulses (π : 32 ns vs. 80 ns in Ref.¹²) with a broader excitation width, and a more central field position $(1220 \text{ mT } vs. 1260 \text{ mT})^{12}$ led to more similar spectra of the native and Sr²⁺substituted S₂ state (Fig. 3D in the main text), as also observed for the native and NH₃-modified S₂ state⁵. This pronounced similarity confirms the structural homogeneity among all three cluster types.

Similar to the high RF region, the RF power may be not entirely uniform also at smaller frequencies such that the ENDOR intensities are not quantitative. This may be the reason why the edge of the ⁵⁵Mn-ENDOR feature ranging from \approx 85 to \approx 95 MHz cannot be correctly reproduced by the simulations (main text Fig. 3).

^{*} It is noted that this behaviour stands in contrast to the effect of RF matching on ⁵⁵Mn-ENDOR resonances observed at a commercial Bruker W-band ENDOR setup in the laboratory of the Bittl group. It is reported that, in the RF range >180 MHz, the peaks intensities are suppressed with increasing radio frequencies and the maxima shifted to lower radio frequencies in the absence of a RF matching network.14. S. Pudollek, Doctoral Thesis, Freie Universität Berlin, 2012.

S7 Electronic structures: exchange couplings and spin states of the BS-DFT models

Table S1 Calculated magnetic parameters for the broken-symmetry (BS) density functional theory (DFT) models of the for S₂ state variants described in the main text (sections 3.1 and 3.3), including total spins *S* of the ground state (GS) and the first excited state (ES) and the energy difference ΔE between these spin states. Listed are also the differences of the electronic exchange coupling constants J_{ij} and energy gaps between the Sr²⁺- and Ca²⁺-containing models Δ (Sr–Ca) and the NH₃- and W1-containing models Δ (NH₃–W1). J_{ij} and ΔE are given in wavenumbers (cm⁻¹).

	Ca	Sr	CaNH ₃	SrNH ₃	$\Delta(Sr$	Δ (Sr–Ca)		₃ -W1)
					W1	NH ₃	Ca	Sr
$J_{\rm CD}\left(J_{12}\right)$	-15.7	-17.6	-15.5	-17.4	-1.9	-2.0	-15.7	-17.6
$J_{\rm BD}\left(J_{13}\right)$	2.0	1.5	5.0	4.7	-0.5	-0.3	2.0	1.5
$J_{\mathrm{AD}}\left(J_{14} ight)$	0.8	0.9	0.2	0.3	0.1	0.1	0.8	0.9
$J_{\rm BC}\left(J_{23}\right)$	23.8	19.3	27.5	22.6	-4.6	-5.0	23.8	19.3
$J_{\mathrm{AC}}\left(J_{24} ight)$	1.9	1.9	1.3	1.4	0.0	0.2	1.9	1.9
$J_{\mathrm{AB}}\left(J_{\mathrm{34}} ight)$	-15.9	-16.0	-11.9	-11.9	-0.2	0.1	-15.9	-16.0
$S_{ m GS}$	1/2	1/2	1/2	1/2			1/2	1/2
S_{ES}	3/2	3/2	3/2	3/2			3/2	3/2
$\Delta E_{ m DFT}$	23.5	26.3	16.8	19.0	+2.8	+2.2	23.5	26.3
ΔE_{exp}	23.5^{12}	26.5 ¹²	30-34 ^{15, 16 a}		+3.0		<u>a</u>	

^{*a*} For the CaNH₃ form of the S₂ state, ΔE was determined on PSII preparations isolated from higher plants (spinach), in contrast to the samples of the Ca and Sr forms, which were isolated from cyanobacterial PSII (*T. elongatus*). Thus, their values are not suited for direct comparison and no difference was calculated.



S8.1 *τ*- and field-dependent Q-Band three-pulse ESEEM spectra

Fig. S4 Q-band three-pulse ESEEM light-minus-dark spectra of the S₂ state Mn₄O₅Ca (A, D), S₂ state Mn₄O₅Sr (B, E) and annealed S₂ state Mn₄O₅Ca–NH₃ (C, F) clusters in PSII isolated from *T. elongatus* at various τ values. (A–C) Time-domain spectra and (D–F) corresponding Fourier transforms. Black solid traces depict the baseline-corrected experimental spectra; superimposing red dashed traces represent simulations based on the spin Hamiltonian formalism as outlined in sections 2.3 in the main text, S3, S4 and S8.4. The optimized parameter sets are listed in Table 3 of the main text and in detail in

Table S2. 'SQ' and 'DQ' refer to the position of single and double-quantum transitions, respectively. For a description of the background subtraction procedure, see section S2. The data from the Mn₄O₅Ca and Mn₄O₅Ca–NH₃ samples at $\tau = 240$ -300 ns were originally reported in Ref.⁵ and reprocessed for this work. Experimental parameters: microwave frequencies: 34.0368 GHz (Ca²⁺), 34.0433 GHz (Sr²⁺), 34.0151 GHz (NH₃); magnetic fields: 1220, 1222 mT; shot repetition time: 1 ms; microwave pulse length (π /2): 12 ns; τ : 220–356 ns (Ca²⁺, Sr²⁺), 200–356 ns (NH₃); ΔT : 100 ns; temperature: 5.2 K.



Fig. S5 Q-band three-pulse ESEEM light-minus-dark spectra of the S₂ state Mn₄O₅Ca (A, D), S₂ state Mn₄O₅Sr (B, E) and annealed S₂ state Mn₄O₅Ca–NH₃ (C, F) clusters in PSII isolated from *T. elongatus* at selected magnetic-field positions across the multiline spectrum. (A–C) Time-domain spectra and (D–F) corresponding Fourier transforms. Black solid traces depict the baseline-corrected experimental spectra; superimposing red dashed traces represent simulations based on the spin Hamiltonian formalism as outlined in sections 2.3 in the main text, S3, S4 and S8.4. The optimized parameter sets are listed in Table 3 of the main text and in detail in Table S2. The labels 'SQ' and 'DQ' refer to the position of single and double-quantum transitions, respectively. For a description of the background subtraction procedure, see section S2. Experimental parameters: microwave frequencies: 34.0368 GHz (Ca²⁺), 34.0433 GHz (Sr²⁺), 34.0151 GHz (NH₃); magnetic fields: 1175–1280 mT (Ca²⁺, Sr²⁺), 1160–1280 mT (NH₃); shot repetition time: 1 ms; microwave pulse length (π /2): 12 ns; τ : 260 ns; ΔT : 100 ns; temperature: 5.2 K.



Fig. S6 (-,+) and (+,+) quadrants of the Fourier-transformed Q-band HYSCORE experimental spectra (A, C, E) and simulations (B, D, F) of the S₂ state Mn_4O_5Ca (A, B), S₂ state Mn_4O_5Sr (C, D) and annealed S₂ state Mn_4O_5Ca -NH₃ (E, F) clusters in PSII isolated from *T. elongatus*, measured at the low field edge of the corresponding Q-band multiline spectra. The labels 'SQ' and 'DQ' indicate the regions of single and double quantum transitions, respectively. The optimized parameter sets for the simulations, as described in sections 2.3 in the main text, S3, S4 and S8.4, are listed in Table 3 of the main text and in detail in Table S2. Experimental parameters: microwave frequencies: 34.0222 GHz (Ca²⁺), 34.0425 GHz (Sr²⁺), 34.0153 GHz (NH₃); magnetic field: 1175 mT; other settings were those given in Fig. 5 in the main article.



Fig. S7 (-,+) and (+,+) quadrants of the Fourier-transformed Q-band HYSCORE experimental spectra (A, C, E) and simulations (B, D, F) of the S₂ state Mn_4O_5Ca (A, B), S₂ state Mn_4O_5Sr (C, D) and annealed S₂ state Mn_4O_5Ca -NH₃ (E, F) clusters in PSII isolated from *T. elongatus*, measured at the high field edge of the corresponding Q-band multiline spectra. The labels 'SQ' and 'DQ' indicate the regions of single and double quantum transitions, respectively. The optimized parameter sets for the simulations, as described in sections 2.3 in the main text, S3, S4 and S8.4, are listed in Table 3 of the main text and in detail in Table S2. Experimental parameters: microwave frequencies: 34.0227 GHz (Ca²⁺), 34.0428 GHz (Sr²⁺), 34.0153 GHz (NH₃); magnetic field: 1260 mT; other settings were those given in Fig. 5 in the main article.



Fig. S8 W-band EDNMR spectra of illuminated **A**) native ¹⁴N-PSII (Mn₄O₅Ca S₂), **B**) Sr²⁺-substituted ¹⁴N-PSII (Mn₄O₅Sr S₂) and **C**) NH₃-modified ¹⁴N-PSII (Mn₄O₅Ca–NH₃ S₂) samples isolated from *T*. *elongatus*. Black solid traces depict the baseline-corrected experimental spectra, red and blue solid traces represent simulations based on the spin Hamiltonian formalism (see sections 2.3 in the main text, S3 and S4). The optimized parameter sets are listed in Table S2. The spectra displayed in each panel S25

were measured or simulated at the low field edge, the center field and the high field edge (top to bottom) of the corresponding W-band multiline EPR spectra (Fig. 3C in the main text). The data from the native S_2 state were originally published in Ref.¹ and were reprocessed to allow comparison to the two chemically modified samples. Experimental parameters: microwave frequencies: 94.011 (A), 93.978 GHz (B), 94.066 GHz (C); magnetic fields: 3.33 T (top), 3.4 T (center), 3.47 T (bottom); shot repetition time: 1.5 ms; microwave pulse length (π): 400 ns; high turning angle pulse length t_{HTA}: 14 µs; τ : 500 ns; temperature: 4.8 K.



Fig. S9 Field-dependent W-band EDNMR spectra of illuminated **A**) native ¹⁵N-PSII ($Mn_4O_5Ca S_2$), **B**) NH₃-modified ¹⁵N-PSII ($Mn_4O_5Ca-NH_3 S_2$) samples isolated from *T. elongatus*. Black solid traces depict the baseline-corrected experimental spectra, red and blue solid traces represent simulations based on the spin Hamiltonian formalism (see sections 2.3 in the main text, S3 and S4). The optimized parameter sets are listed in Table S2. The spectra displayed in each panel were measured or simulated at the low field edge, the center field and the high field edge (top to bottom) of the corresponding W-band multiline EPR spectra (Fig. 3C in the main text). Experimental parameters: microwave frequencies: 94.022 GHz (A), 93.996 GHz (B); magnetic fields: 3.33 T (top), 3.4 T (center), 3.47 T (bottom); shot repetition time: 0.5 ms; microwave pulse length (π): 160 ns; t_{HTA}: 8 µs; τ : 500 ns; temperature: 4.8 K.

Both the ¹⁴N and ¹⁵N spectra are highly similar for the native, Sr^{2+} -substituted and NH₃-modified S₂ states. The three systems exhibit identical orientation dependencies, with the clearly largest splitting at the central field position ($g \approx 1.98$) and smaller splittings at the low- and high-field edges ($g \approx 2.02$ and $g \approx 1.94$, respectively). This behaviour is shown by both the ¹⁴N and ¹⁵N signals of the His332 imino-N. At the outer magnetic-field positions, the hyperfine splittings are approximately of the same size. The general similarity of the ¹⁴N orientation selectivity to that of the ¹⁵N signals results from the fact that the hyperfine coupling is the dominant electron-nuclear interaction and the magnitude of the NQI is considerably smaller. Despite the similar overall field-dependence, there are differences in the exact positions of the peaks, most prominent for the double-quantum transitions, at a certain magnetic field between the three variants of the S₂ state.

S8.4 Magnetic parameters of the His332 imino-¹⁴N interactions with the S₂ state OEC forms

Table S2 Effective/projected ¹⁴N hyperfine and NQI tensors in MHz for the interaction of the His332 imino-N with the Mn_4O_5Ca , Mn_4O_5Sr and annealed Mn_4O_5Ca –NH₃ clusters in the S₂ state in PSII from *T. elongatus* and parameters from previous studies on various species. The Q-band ESEEM/HYSCORE (Figs. 5 in the main text, S4, S5, S6 and S7) and the W-band EDNMR (Figs. S8, S9) simulations employed two different *A* tensors for a given spin system, while the NQI tensor and the Euler angle rotations of the hyperfine and NQI tensor were identical for the two frequencies.

S ₂ state	Method	$ A_1 $	$ A_2 $	$ A_3 $	$ A_{\rm iso} ^a$	$A_{dip}{}^b$	$A_{\eta}{}^{c}$	$ e^2 Qq/h $	η^c
	Q-Band ^d	5.6	8.4	7.2	7.1	0.75	0.81		
Native	W-band ^d	3.2	9.2	6.7	6.3	1.59	0.80	1.97	0.75
	BS-DFT ^e	4.6	5.9	6.8	5.8	0.59	0.74	1.65	0.91
	Q-Band ^d	5.9	8.5	7.4	7.3	0.69	0.83	1.00	0.70
Sr ²⁺ -substituted	W-band ^d	3.4	9.6	6.8	6.6	1.58	0.87	1.98	0.79
	$BS-DFT^{e}$	4.7	6.1	6.8	5.8	0.57	0.61	1.65	0.91
	Q-Band ^d	5.7	8.6	7.3	7.2	0.75	0.89	1.00	0.90
NH ₃ -modified	W-band ^d	3.5	9.1	6.6	6.4	1.45	0.86	1.90	0.80
	$BS-DFT^e$	4.7	6.1	7.5	6.1	0.71	0.99	1.68	0.88
Native, spinach ¹⁷	X-, P-, K _a -band	6	.3, 7.8, 7	.8	7.3	0.5	0	1.98	0.84
Native, <i>Synechocystis</i> sp. PCC 6803 ¹⁸	K _a -, Q-band ^f	5.4	5, 7.15, 8	8.25	6.95	0.75	0.73	1.98	0.82
Native ¹	W-band ^g	3.8	7.7	6.2	5.9	1.1	0.71	0	0

^{*a*} A_{iso} is defined as the average of the principal components of the hyperfine tensor: $A_{iso} = (A_1 + A_2 + A_3)/3$. ^{*b*} A_{dip} is defined in terms of T_1 , T_2 , and T_3 as $A_{dip} = (T_1 + T_2)/2 = -T_3/2$. ^{*c*} The rhombicity is defined by A_{η} or $\eta = (T_1 - T_2)/T_3$, respectively. T_1 , T_2 , and T_3 represent the three principal components of the hyperfine tensors minus A_{iso} and of the NQI tensors and are labeled such that $|T_1| \le |T_2| \le |T_3|$. ^{*d*} The Euler rotation angles $[\alpha, \beta, \gamma]$ are $[0, 45, 0]^\circ$, $[0, 45, 0]^\circ$ and $[0, 44, 0]^\circ$ for the *A* tensors and $[20, -57, 0]^\circ$, $[18, -54, 0]^\circ$ and $[16, -60, 0]^\circ$ for the NQI tensors of the Mn₄O₅Ca, Mn₄O₅Sr and Mn₄O₅Ca–NH₃ clusters,

respectively. ^{*e*} Their calculated orientations are such that the smallest, medium and large effective components are aligned approximately (angular deviation < 6°) along the Mn_{D1}–His332, the Mn_{D1}-O3 and the Mn_{D1}–Asp342, respectively (Fig. S10, main text Fig. 1). By definition, the large components along the Jahn-Teller axis were assigned to A_3 and, by inspection, the others to A_1 and A_2 . ^{*f*} The Euler rotation angles [α , β , γ] of the NQI tensor are [-30, 0, 40]°. ^{*g*} Euler rotation angles [α , β , γ] of the hyperfine tensor were [0, 30, 0]°.

A simultaneous fitting of all Q-band three-pulse ESEEM (Figs. S4, S5) and HYSCORE (Figs. 5 in the main text, S6 and S7) spectra and W-band ¹⁴N- and, if available, ¹⁵N-EDNMR spectra (Figs. S8 and S9) of the native, the Sr^{2+} -substituted and the NH₃-modified S₂ state was performed using the spin Hamiltonian formalism (see Materials and Methods section 2.3 and sections S3 and S4). Only one nitrogen nucleus was included representing the coordinating imino-N in the imidazole ring of His332. Non-coordinating nitrogens do not contribute significantly to the ESEEM and HYSCORE modulations and the EDNMR spectra (see also Figs. S8 and S9).^{1, 17, 19} As the relative intensities of single- and double-quantum transition lines in EDNMR experiments are highly dependent on an experimental parameter, namely the high turning angle (HTA) pulse, single- and double-quantum transitions were calculated and normalized separately in the simulations, as in Rapatskiy *et al.*¹ and Pérez Navarro *et al.*⁵. The fitted effective ¹⁴N A and NQI tensors are listed in Table S2. In case of the ¹⁵N EDNMR spectra, the A tensor components were scaled by the ratio of the nuclear *g* values of ¹⁴N and ¹⁵N (and no NQI is effective). The effective *G* tensors used were the same as those determined by the EPR and ⁵⁵Mn-ENDOR simulations (Table 1 in the main text).

In simulations where the entire Q-band ESEEM/HYSCORE dataset was included, a single, consistent parameter set could be obtained. The fitted hyperfine and NQI parameters of all three S_2 state variants are very similar to those reported in higher plant and mesophilic cyanobacterial (*Synechocystis* sp. PCC 6803) PSII by the Britt laboratory^{17, 18} (Table S2). These simulations though do not constrain the orientation of the hyperfine tensor orientations relative to the *G* matrix. The inclusion of the high-S30

frequency W-band EDNMR data allows the relative tensor orientations to be ascertained. However, the hyperfine tensors found to reproduce the field dependence of the W-band EDNMR dataset do not reproduce the Q-band ESEEM and HYSCORE data but instead comprise a smaller isotropic and a larger dipolar component. As the blue solid traces in Figs. S8 and S9 show, the splitting of the peaks in the W-band EDNMR spectra is overestimated when employing the hyperfine tensors fitted to the Q-band ESEEM and HYSCORE data, already to a smaller extent at the center field and more drastically at the edge position. Since our simulations of the W-band EDNMR signals now explicitly include the NQI term, the omission of this term cannot be the reason for this apparent mismatch. A rationale for this difference is given in the main text section 3.4. Despite the differences of the size of the dipolar component A_{dip} of the nitrogen hyperfine interaction between the Q- and W-band simulations, for all three S₂ state variants, their rhombicities A_{η} are very similar.

For the three forms of the S_2 state, the hyperfine tensors were required to be rotated about -45° around the y axis, relative to the orientation of the effective G tensors, which resulted to be rhombic from the simulations of the EPR/⁵⁵Mn ENDOR spectra in this work (main text section 3.2). This is similar to the simulation of the ¹⁴N-EDNMR spectra at W-band of the native S₂ state in Ref.¹. This rotation results from the fact that approximately the same peak splittings are present in the W-band EDNMR spectra recorded at the edge positions of the S_2 multiline, corresponding to the x and z axes in the G tensor frame. Thus, the hyperfine coupling is expected to be small along G_x and G_z and large along G_y . However, the effective ¹⁴N/¹⁵N hyperfine tensor cannot be axial, as inferred from the ESEEM and HYSCORE spectra. Hence, it is supposed that the A tensor of the imino- 14 N/ 15 N and the molecular G tensor are not collinear. A β angle rotation in the xz plane (Fig. S10) allows the EDNMR data to be fit employing a rhombic hyperfine tensor, as noted earlier in Ref.¹. The simulations also afforded rotations of the NQI tensor around the z axis ($\alpha = 16$ to 20°) and the y' axis ($\beta = -54$ to -60°). Upon a switch of the values of A_1 and A_3 and use of $\beta = 45^\circ - 90^\circ = -45^\circ$, generating the same simulation traces, it becomes obvious that the orientations of NQI and hyperfine tensors are relatively similar, as observed in previous simulations of K_a- and Q-band three-pulse ¹⁴N and ¹⁵N-ESEEM data of this His332 imino-N.¹⁸



Fig. S10 Proposed orientations of the His332 imino-¹⁴N/¹⁵N and ¹⁴NH₃ hyperfine tensors relative to the fine structure tensor of the Mn_{D1}^{III} ion *d* and the molecular *G* frame in a schematic model of the Mn_4O_5Ca –NH₃ cluster. a_1 , d_1 and G_z define the unique tensor axis, 'JT' denotes the Jahn-Teller axis of Mn_{D1}^{III} .



Fig. S11 X-band three-pulse ESEEM light-minus-dark spectra of ¹⁴NH₃-modified native ¹⁵N-PSII, ¹⁵NH₃-modified native ¹⁴N-PSII and ¹⁴NH₃-modified Sr²⁺-substituted ¹⁴N-PSII (top to bottom) samples isolated from *T. elongatus* in the annealed S₂ state. **A)** Time-domain spectra and **B**) corresponding Fourier transforms. Black traces depict the baseline-corrected experimental spectra (see section S2); superimposing red traces represent simulations based on the spin Hamiltonian formalism (see sections 2.3 in the main text, S3 and S4). The optimized parameter sets are listed in Table S3. The ¹⁵N-PSII-Ca ¹⁴NH₃ and ¹⁴N-PSII-Ca ¹⁴NH₃ data were originally presented in Pérez Navarro *et al.*⁵ and reprocessed for this work. Experimental parameters: microwave frequencies: 9.680 GHz, 9.674 GHz, 9.684 GHz, 9.681 GHz (top to bottom); magnetic field: 333 mT; shot repetition time: 8.16 ms; microwave pulse length (π /2): 8 ns; τ : 136 ns (A), average of experiments with 136, 152, 168, 184 ns (B); ΔT : 64 ns; temperature: 4.3 K.

Table S3 Fitted (X-band three-pulse ESEEM, Fig. S11) and calculated effective/projected ¹⁴N hyperfine and NQI tensors, listed as absolute values in MHz, for the electron-nuclear coupling of the NH₃ bound in the annealed $Mn_4O_5Ca-NH_3$ and $Mn_4O_5Sr-NH_3$ S₂ state clusters in PSII from *T. elongatus* and, from earlier studies, higher plant spinach.

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S_2 state	Method	$ A_1 $	$ A_2 $	$ A_3 $	$ A_{\rm iso} ^a$	$A_{\rm dip}$	A_{η}^{c}	$ e^2Qq/h $	η^{c}
Mn ₄ O ₅ Ca–NH ₃	ESEEM	1.69	2.76	2.62	2.36	0.33	0.22	1.52	0.47
	BS-DFT	3.97	2.01	2.04	2.68	-0.65	0.02	0.94	0.87
Mn ₄ O ₅ Sr–NH ₃	ESEEM	1.81	2.72	2.59	2.37	0.28	0.23	1.58	0.45
	BS-DFT	3.87	2.07	2.10	2.68	-0.59	0.03	0.93	0.87
Mn ₄ O ₅ Ca–NH ₃ , spinach ²⁰	ESEEM	1.89	2.49	2.49	2.29	0.20	0.0	1.61	0.59

^{*a*} A_{iso} is defined as the average of the principal components of the hyperfine tensor: $A_{iso} = (A_1 + A_2 + A_3)/3$. ^{*b*} A_{dip} is defined in terms of T_1 , T_2 , and T_3 as $A_{dip} = (T_1 + T_2)/2 = -T_3/2$. ^{*c*} The rhombicity is defined by A_{η} or $\eta = (T_1 - T_2)/T_3$, respectively. T_1 , T_2 , and T_3 represent the three principal components of the hyperfine tensors minus A_{iso} and of the NQI tensors and are labeled such that $|T_1| \le |T_2| \le |T_3|$.

Three-pulse ESEEM experiments were performed at X-band on ¹⁴NH₃/¹⁵NH₃-modified (annealed), Ca²⁺-and Sr²⁺-containing, wild-type and all-¹⁵N-labeled PSII samples in the NH₃-treated S₂ state. Fig. S11 depicts light-minus-dark-corrected time-domain (Fig. S11A) and, to minimize spectral artifacts, *r*-averaged frequency-domain (Fig. S11B) spectra at 4.8 K of ¹⁴NH₃-modified native ¹⁵N-PSII, ¹⁵NH₃-modified native ¹⁴N-PSII, ¹⁴NH₃-modified native ¹⁴N-PSII, ¹⁴NH₃-modified native ¹⁴N-PSII, ¹⁴NH₃-modified native ¹⁴N-PSII and ¹⁴NH₃-modified Sr²⁺-substituted ¹⁴N-PSII (top to bottom). At X-band frequencies, the echo modulations are dominated by the nitrogen hyperfine interaction of the bound NH₃ as it meets the cancellation condition ($A = 2v_n$). Importantly, the His332 imino-N interaction is suppressed as at X-band. Resonances from ¹⁴N nuclei (I = 1), which exhibit significant NQI contributions in contrast to the ¹⁵N nucleus ($I = \frac{1}{2}$), appear more prominent in the three-pulse ESEEM data than those from ¹⁵N ligands. Thus, the ¹⁴NH₃-modified native ¹⁵N-PSII data are dominated by the ¹⁴NH₃ interactions as compared to the ¹⁵N His332 resonances, while all ¹⁴N-PSII spectra show a broad His332 imino-¹⁴N resonance centered at ≈4.6 MHz in the Fourier-transformed spectrum.⁵

Spectral simulations of the X-band time-domain data were performed as described in the Materials and Methods section 2.3 and sections S3 and S4. They also included the ligating imino-¹⁴N or -¹⁵N nucleus of His332, represented by the fitted Q-band parameters, and contributions from ¹H nuclei. The ¹H resonances, not displayed in the Fourier transforms, are centered at \approx 14.2 MHz and were largely suppressed at a τ length of 136 ns.

The presented BS-DFT calculations confirm the small hyperfine rhombicity, however, yielding a negative dipolar hyperfine component with the unique component being the largest. The non-axiality of the electric field gradient, inferred from the large asymmetry parameter $\eta = 0.47$ of the NQI and reproduced by the BS-DFT computations, is attributed to a non-axial H-bonding geometry (main text section 4.1.2b, Fig. 7). In the original work by Britt *et al.*²⁰, the large η was proposed not to arise from a terminal NH₃ but rather from a less symmetric amido (NH₂) bridge between two Mn and/or the Ca²⁺ ion.



S10.1 W-band ¹⁷O-ELDOR-detected NMR experiments

Fig. S12 Single-quantum (left) and double-quantum (right) regions of the ¹⁷O-EDNMR spectra of the native (Ca) the Sr^{2+} -substituted (Sr), the NH₃-annealed (CaNH₃) and the Sr^{2+} -substituted NH₃-annealed (SrNH₃) S₂ states in PSII samples isolated from *T. elongatus*. The double-quantum envelopes are presented on a 4 times expanded vertical scale as compared to the single quantum resonances. Black solid traces show the background-corrected experimental spectra; superimposing red dashed traces represent simulations based on the spin Hamiltonian formalism as outlined in sections 2.3 in the main text, S3, S4. Coloured dashed lines represent a decomposition of the simulation showing contributions

from the individual ¹⁴N and ¹⁷O nuclei. Black dashed lines, visualizing the shift of the fitted single- and double-quantum transition peaks, highlight the decrease of the strong ¹⁷O interaction, assigned to the μ -oxo bridge O5, upon substitution of the Ca²⁺ for a Sr²⁺ ion. The optimized parameter sets are listed in Table S4. Same as for the ¹⁴N- and ¹⁵N-EDNMR signals, the single- and double-quantum resonances of each ¹⁷O species were weighted and normalized individually. In the simulations, the double-quantum peaks ν_{α} and ν_{β} of the individual ¹⁷O species were required to be equal, unlike in Refs.^{1, 5}, where an intensity imbalance was allowed for. The data from the NH₃-treated S₂ state were originally published in Ref.¹ and were reprocessed to allow comparison to the other S₂ state forms. Experimental parameters: microwave frequencies: 93.988 (Ca), 94.033 GHz (Sr), 94.069 GHz (CaNH3), 93.964 GHz (SrNH3); magnetic field: 3.4 T; shot repetition time: 1.5 ms; microwave pulse length (π): 400 ns; t_{HTA}: 14 µs; τ : 500 ns; temperature: 4.8 K..



Fig. S13 Effect of Ca²⁺/Sr²⁺ exchange on the single-quantum (left) and double-quantum (right) envelopes of the ¹⁷O-EDNMR spectra of the not NH₃-treated (top) and NH₃-annealed (bottom) S₂ states in PSII samples isolated from *T. elongatus*. The blue traces depict the Ca²⁺-containing Mn₄O₅Ca and Mn₄O₅Ca-NH₃ clusters, red traces represent the Sr²⁺-containing Mn₄O₅Sr and Mn₄O₅Sr-NH₃ clusters. The double-quantum envelopes are presented on a 4.5 times expanded vertical scale as compared to the single quantum resonances. They were smoothed using a 9-point moving average and normalized with respect to the high-frequency doublet peak around 43 MHz for better comparability. As pointed out by the horizontal arrows, Sr²⁺ substitution results in a systematic narrowing of the single- and double quantum envelopes in both the S₂ states without and with NH₃ bound to the Mn cluster. The vertical arrows mark the maximum of the underlying ν_β peaks of the His332 imino-¹⁴N, which prevent the low-frequency edges of the ¹⁷O single-quantum envelopes and thus their differences from being resolved. Experimental parameters: see Fig. S12.

Table S4 Fitted effective ¹⁷O hyperfine tensors, listed as absolute values in MHz, from W-band EDNMR experiments (Fig. 6 in the main text and Fig. S12) for the electron-nuclear coupling of the oxygen species exchangeable in the S₁ state with the Mn₄O₅Ca, Mn₄O₅Sr, Mn₄O₅Ca–NH₃ and Mn₄O₅Sr–NH₃ S₂ state clusters in PSII from *T. elongatus*. A_1 , A_2 and A_3 are the principal components of the hyperfine tensor, which are not assigned to the principal axes of the coordinate system defined by the *G* tensor.

S ₂ state	Oxygen	$ A_1 $, $ A_2 $, $ A_3 $	$ A_{\rm iso} ^a$	$A_{dip}{}^b$	$A_{\eta}{}^{c}$
all	matrix	2.1, 0.2, 2	1.4	0.6	0.08
Mn ₄ O ₅ Ca	W2	5.1, 5.1, 3.3	4.5	0.6	0.08
	05	10.7, 5.3, 13.1	9.7	2.2	0.55
Mn ₄ O ₅ Sr	W2	5.1, 5.1, 3.3	4.5	0.6	0.08
	05	10.2, 4.8, 12.6	9.2	2.2	0.55
Mn ₄ O ₅ Ca–NH ₃	W2	3.7, 3.7, 1.9	3.1	0.6	0.08
	05	8.0, 2.6, 10.4	7.0	2.2	0.55
Mn ₄ O ₅ Sr–NH ₃	W2	3.7, 3.7, 1.9	3.1	0.6	0.08
	05	7.5, 2.1, 9.9	6.5	2.2	0.55

^{*a*} A_{iso} is defined as the average of the principal components of the hyperfine tensor: $A_{iso} = (A_1 + A_2 + A_3)/3$. ^{*b*} A_{dip} is defined in terms of T_1 , T_2 , and T_3 as $A_{dip} = (T_1 + T_2)/2 = -T_3/2$. ^{*c*} The rhombicity is defined by A_{η} or $\eta = (T_1 - T_2)/T_3$, respectively. T_1 , T_2 , and T_3 represent the three principal components of the hyperfine tensors minus A_{iso} and of the NQI tensors and are labeled such that $|T_1| \le |T_2| \le |T_3|$.

S10.2 X-band CW EPR experiments in the absence and presence of H₂¹⁷O



Fig. S14 X-band CW EPR spectra of the Sr²⁺-substituted S₂ state in PSII samples in the absence (black) and presence (red) of H₂¹⁷O showing no line broadening upon ¹⁷O exchange. The spectrum in the not H₂¹⁷O -enriched buffer was taken from Cox *et al.*¹². In the spectrum of the H₂¹⁷O-exchanged PSII sample, the Y_D• signal centered at about $g \approx 2$ was removed for clarity of presentation; the underlying comparatively narrow signal centered at $g \approx 1.66$ originates from the semiquinone-iron in the Q_A⁻Fe²⁺Q_B⁻ state.^{21, 22} Experimental parameters: microwave frequencies: 9.4213 GHz (no ¹⁷O); 9.4989 GHz (with ¹⁷O); microwave power: 20 mW; modulation amplitude: 25 G; time constant: 82 ms; temperature: 8.6 K.

S11 References

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