

Supporting Information

# Proton Isomers Rationalize the High- and Low-Spin Forms of the S<sub>2</sub> state Intermediate in the Water-Oxidizing Reaction of Photosystem II.

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## Methodology

### Computational details

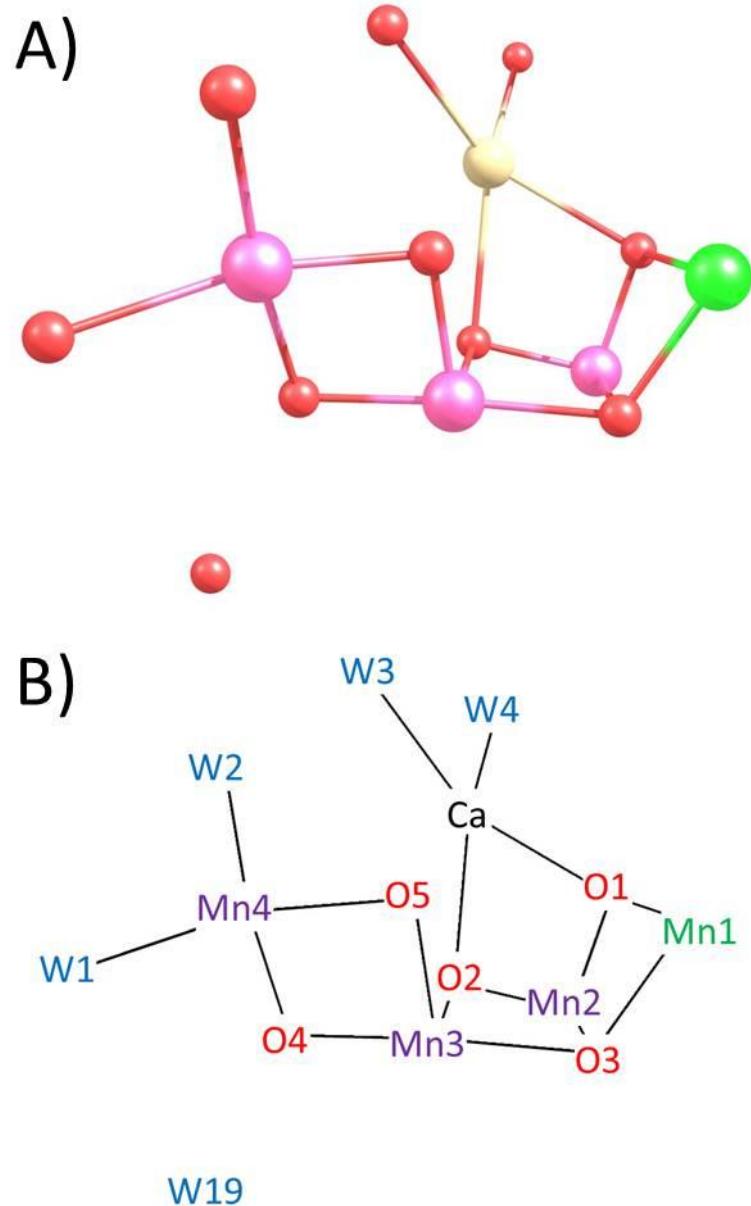
Calculations were performed using ORCA 4<sup>1</sup> and the computational procedure used has been described previously.<sup>2</sup> All models were geometry optimised into their respective high spin states using the BP86 functional.<sup>3,4</sup> The zeroth-order regular approximation (ZORA) Hamiltonian was applied to include scalar relativistic effects.<sup>5-7</sup> ZORA versions of the def2-SVP basis sets were used for C and H atoms. All other atoms used ZORA versions of the def2-TZVP basis set with f functions removed.<sup>8</sup> The resolution of identity approximation (RI-J) for coulomb integrals, along with the decontracted general Weigend auxiliary basis sets were used.<sup>9-11</sup> Dispersion corrections proposed by Grimme along with Becke-Johnson damping (D3BJ) were included.<sup>12,13</sup> All calculations included the conductor-like polarizable continuum model (CPCM) with a dielectric constant  $\epsilon = 8.0$  in line with previous studies.<sup>14,15</sup> Integration grids were increased (Grid6 and IntAcc 6 in ORCA convention) and tight SCF convergence criteria applied. Throughout optimisation calculations all terminal carbon atoms were constrained. The Heisenberg exchange coupling constants were calculated using the

broken symmetry DFT (BS-DFT) methodology proposed by Pantazis *et al.*<sup>14,16</sup> For BS-DFT calculations the hybrid meta-GGA TPSSh functional was used. The chain of spheres (RIJCOSX) approximation to exact exchange was applied along with the same decontracted auxillary basis sets involved in geometry optimization calculations.<sup>17,18</sup> The ZORA versions of the def2-TZVP basis set with f functions removed was used for all atoms.<sup>8</sup> The ‘flipspin’ feature of ORCA was used to construct initial BS guesses.<sup>19</sup> Convergence to the correct BS and HS states in all calculations was confirmed by examination of the calculated Mulliken spin populations. Spin ladder calculations were performed using the ‘orca\_eca’ module within ORCA. For all single point energy calculations the same method as described for BS-DFT calculations was used with alternative functionals (BP86, B3LYP, TPSS0 and TPSSh).

## Model systems

All starting models were generated from the S<sub>2</sub> XFEL crystal structure (PDB: 6DHF)<sup>20</sup> and geometry optimised into the S<sub>2</sub> state. All models used the HS oxidation state of (Mn<sup>III</sup>)(Mn<sup>IV</sup>)<sub>3</sub> as used in previous studies.<sup>21</sup> The models contain seven directly coordinated amino acids, six of which are from the D1 protein chain (Asp-170, Glu-189, His-332, Glu-333, Asp-342, Ala-344) and one from the CP43 protein chain (Glu-354). The following second sphere residues were also included (all are located in the D1 protein chain unless stated otherwise): Asp-61, Tyr-161(Y<sub>z</sub>), Gln-165, Ser-169, His-190, Asn-298, His-337 and CP43-Arg-357, along with the partial backbone of Glu-329 which hydrogen bonds to His-332. All terminal carbon atoms were constrained throughout the calculations. Each model contains four water molecules directly coordinated to the WOC, two bound to Mn<sub>4</sub> (W1 and W2) and two bound to Ca (W3 and W4), along with sixteen crystallographic water molecules. In the O4 model all bridging oxygen atoms are in  $\mu$ -oxo (O<sup>2-</sup>). In the O4H and O5H models, O4 and O5 are modelled as  $\mu$ -hydroxo (OH) ligand between Mn<sub>4</sub> and Mn<sub>3</sub> respectively whilst keeping all other bridging oxygen atoms as  $\mu$ -oxo (O<sup>2-</sup>). Coordinated

water ligands W3 and W4 were in the aquo form, with W2 as a hydroxo ligand and W1 as an aquo or hydroxo depending on model.



**Figure S1:** A) The WOC structure and labelling described in the main text. The open cubane is maintained in all models. Hydrogens have been excluded for clarity. Colour coding: MnIII (green), MnIV (pink), oxygen (red) and calcium (white). B) The commonly referred atom names as described in the main text. Ligand and crystallographic waters are shown in blue to distinguish from bridging oxygens which are shown in red.

## Mulliken Spin populations

**Table S1:** The Mulliken spin populations of each manganese centre (Mn1-4) are shown, confirming the oxidation state  $(\text{Mn}^{\text{III}})(\text{Mn}^{\text{IV}})_3$  for all models.

	Mn1	Mn2	Mn3	Mn4
O4	3.90	2.90	2.80	2.89
O4H	3.90	2.91	2.85	2.87
O5H	3.89	2.91	2.82	2.88

## References

- (1) Neese, F. Software Update: The ORCA Program System, Version 4.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2018**, 8 (1), e1327.
- (2) Corry, T. A.; O'Malley, P. J. Evidence of O–O Bond Formation in the Final Metastable  $\text{S}_3$  State of Nature's Water Oxidizing Complex Implying a Novel Mechanism of Water Oxidation. *J. Phys. Chem. Lett.* **2018**, 6269–6274.
- (3) Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A* **1988**, 38 (6), 3098–3100.
- (4) Perdew, J. P. Density-Functional Approximation for the Correlation Energy of the Inhomogeneous Electron Gas. *Phys. Rev. B* **1986**, 33 (12), 8822–8824.
- (5) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. Relativistic Regular Two-component Hamiltonians. *J. Chem. Phys.* **1993**, 99 (6), 4597–4610.
- (6) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. Relativistic Total Energy Using Regular Approximations. *J. Chem. Phys.* **1994**, 101 (11), 9783–9792.
- (7) van Wüllen, C. Molecular Density Functional Calculations in the Regular Relativistic Approximation: Method, Application to Coinage Metal Diatomics, Hydrides, Fluorides and Chlorides, and Comparison with First-Order Relativistic Calculations. *J. Chem. Phys.* **1998**, 109 (2), 392–399.
- (8) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, 7 (18), 3297–3305.
- (9) Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. Auxiliary Basis Sets to Approximate Coulomb Potentials. *Chem. Phys. Lett.* **1995**, 240 (4), 283–289.
- (10) Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. Auxiliary Basis Sets for Main Row Atoms and Transition Metals and Their Use to Approximate Coulomb Potentials. *Theor. Chem. Accounts Theory, Comput. Model. (Theoretica Chim. Acta)* **1997**, 97 (1–

- 4), 119–124.
- (11) Weigend, F. Accurate Coulomb-Fitting Basis Sets for H to Rn. *Phys. Chem. Chem. Phys.* **2006**, *8* (9), 1057–1065.
- (12) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate *Ab Initio* Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132* (15), 154104.
- (13) Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the Damping Function in Dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **2011**, *32* (7), 1456–1465.
- (14) Pantazis, D. A.; Ames, W.; Cox, N.; Lubitz, W.; Neese, F. Two Interconvertible Structures That Explain the Spectroscopic Properties of the Oxygen-Evolving Complex of Photosystem II in the S<sub>2</sub> State. *Angew. Chemie Int. Ed.* **2012**, *51* (39), 9935–9940.
- (15) Cox, N.; Retegan, M.; Neese, F.; Pantazis, D. A.; Boussac, A.; Lubitz, W. Electronic Structure of the Oxygen-Evolving Complex in Photosystem II Prior to O-O Bond Formation. *Science* **2014**, *345* (6198), 804–808.
- (16) Pantazis, D. A.; Orio, M.; Petrenko, T.; Zein, S.; Bill, E.; Lubitz, W.; Messinger, J.; Neese, F. A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transition-Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystem II. *Chem. - A Eur. J.* **2009**, *15* (20), 5108–5123.
- (17) Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. Comparative Assessment of a New Nonempirical Density Functional: Molecules and Hydrogen-Bonded Complexes. *J. Chem. Phys.* **2003**, *119* (23), 12129–12137.
- (18) Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. Efficient, Approximate and Parallel Hartree-Fock and Hybrid DFT Calculations. A “chain-of-Spheres” Algorithm for the Hartree-Fock Exchange. *Chem. Phys.* **2009**, *356* (1–3), 98–109.
- (19) Neese, F. The ORCA Program System. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2* (1), 73–78.
- (20) Kern, J.; Chatterjee, R.; Young, I. D.; Fuller, F. D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A. S.; Alonso-Mori, R.; et al. Structures of the Intermediates of Kok’s Photosynthetic Water Oxidation Clock. *Nature* **2018**, *1*.
- (21) Beal, N. J.; Corry, T. A.; O’Malley, P. J. Comparison between Experimental and Broken Symmetry Density Functional Theory (BS-DFT) Calculated Electron Paramagnetic Resonance (EPR) Parameters of the S<sub>2</sub> State of the Oxygen-Evolving Complex of Photosystem II in Its Native (Calcium) and Strontium-Substituted Form. *J. Phys. Chem. B* **2017**, *121* (50), 11273–11283.

## Coordinates

### O4

Ca	-32.66270677387632	39.74318578787990	362.02512687989110
O	-33.17997282618111	39.56067570731263	364.35656907825273
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