

Effect of $\text{Ca}^{2+}/\text{Sr}^{2+}$ Substitution on the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II: A Combined Multifrequency EPR, ^{55}Mn -ENDOR, and DFT Study of the S_2 State [*Journal of the American Chemical Society* **2011**, *133*, 3635–3648 DOI: 10.1021/ja110145v]. Nicholas Cox,* Leonid Rapatskiy, Ji-Hu Su, Dimitrios A. Pantazis, Miwa Sugiura, Leonid Kulik, Pierre Dorlet, A. William Rutherford, Frank Neese, Alain Boussac, Wolfgang Lubitz,* and Johannes Messinger*

It came to our attention that we neglected to reference the work of Teutloff et al.,¹ which tentatively assigned the position of the Mn^{III} ion in the S_2 state of the water-oxidizing complex of *Thermosynechococcus elongatus*, as deduced from ^{55}Mn -ENDOR studies on PSII single crystals. Our present analysis and the Teutloff et al.¹ report are in agreement and as such, together with recent theoretical calculations² of EPR parameters, further strengthen the conclusion that the model for the structure of the water-oxidizing complex in the S_2 state proposed by Siegbahn provides an excellent basis for describing all available magnetic resonance data. Furthermore, with minor adjustments, this model appears broadly consistent with new crystallographic data³ of PSII at 1.9 Å resolution recently published in Nature (PDB 3ARC).

■ REFERENCES

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