University of Windsor

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

CEMWOQ 3

3rd Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec

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Sample Abstract

Title (entered in title box):

Multi-Frequency EPR Analysis of Dipolar and Exchange Interactions Between Managese and Tyrosine In The S2 Yz State of Photosystems II

Authors and author locations (entered in authors box and author locations box):

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Abstract (entered in abstract box):

Acetate-inhibited photosystem II, upon room temperature illumination, exhibits a 240 G wide X-band EPR signal at 10 K.1 This EPR signal arises from an interaction between the S2 state of the Mn4 cluster and an oxidized tyrosine residue, Yz.2 In the present study, the exchange and dipolar interactions between the two paramagnetic species are simulated at X and Q-band frequencies utilizing second-order perturbation theory.3 The positions and relative intensities of the hyperfine lines in the S = ••• S2 -state multiline EPR signal are accurately simulated by including g-anisotropy and four sets of axially symmetric 55Mn hyperfine tensors. These parameters are then used to simulate the dipolar and exchange interactions giving rise to the broad experimental S2 Yz EPR signal at X and Q-band frequencies. A precise distance determination between the Mn4 Cluster and Yz in the O2-evolving complex better enables us to elucidate the direct involvement of Yz in water-oxidation chemistry. Supported by NIH GM32715 and GM36442 (Yale) and NIH GM21156 (Denver).
1. Boussac and Rutherford, *Biochem.,* **1988**, *27*, 3476.
2. Tang et al., *J. Amer. Chem. Soc.,* **1996**, *118*, 7638.
3. Eaton et al., *J. Magn. Res.,* **1983**, *52*, 435.