



61st Annual Rocky Mountain Conference on Magnetic Resonance
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Abstract Submission Instructions

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Sample abstract:

Title (entered in title box):

Multi-Frequency EPR Analysis of Dipolar and Exchange Interactions Between Manganese and Tyrosine In The $S_2 Y_z$ State of Photosystems II

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

K.V. Lakshmi,¹ Sandra S. Eaton,² George H. Johansson,³ and Helmut Schmidt.⁴

1. Yale University, Department of Chemistry, New Haven, CT 06520-8107

2. University of Denver, Department of Chemistry, Denver, CO 80208-2436

3. University of Southern Denmark, Department of Physics and Chemistry, 5230 Odense M, Denmark

4. University of Leipzig, Institute for Experimental Physics II, Leipzig, 04103 Germany

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 S_2 state of the Mn_4 cluster and an oxidized tyrosine residue, Y_z .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 $S = \frac{1}{2} S_2$ -state multiline EPR signal are accurately simulated by including g-anisotropy and four sets of axially symmetric ^{55}Mn hyperfine tensors. These parameters are then used to simulate the dipolar and exchange interactions giving rise to the broad experimental $S_2 Y_z$ EPR signal at X and Q-band frequencies. A precise distance determination between the Mn_4 cluster and Y_z in the O₂-evolving complex better enables us to elucidate the direct involvement of Y_z 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.