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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

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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 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.