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**Single Crystal ESEEM Spectroscopic and Computational Chemical Analysis of Coupled  $^{17}\text{O}$  in Copper-Doped Enriched Tutton Salt.** M.J. Colaneri, J. Vitali, J. Peisach, Dept. of Chemistry & Physics, SUNY at Old Westbury, Old Westbury, NY 11568, Dept. of Physics, Cleveland State Univ., Cleveland, OH 44114 and Dept. of Physiology & Biophysics, Albert Einstein College of Medicine, Bronx, NY 10461

Electron Spin-Echo Envelope Modulation (ESEEM) spectroscopic studies and quantum mechanical calculations were performed on  $\text{Cu}^{+2}$ -doped  $^{17}\text{O}$ -enriched potassium zinc sulfate hexahydrate (tutton salt) crystals in order to measure the  $^{17}\text{O}$  hyperfine and quadrupole coupling tensors from  $\text{H}_2^{17}\text{O}$  weakly bound to copper. This analysis extends our earlier ESEEM results on tutton crystal samples. The obtained  $^{17}\text{O}$  hyperfine tensor can be modeled to arise from a combination of classical dipole-dipole components, producing a significantly rhombic form. The measured  $^{17}\text{O}$  quadrupole tensor is in the range of nuclear quadrupole interactions reported in studies of  $^{17}\text{O}$ -water salt hydrates. Chemical computations were carried out with the Gaussian 03 suite using various model chemistries. Theoretical coupling tensors derived from these models will be compared to those experimentally determined. The analysis of small coupling interactions from distant  $\text{H}_2^{17}\text{O}$  have important implications in studies of copper enzymes where substrates have been proposed to displace weakly bound water in the active site.