## SUPPORTING INFORMATION



**Figure S1.** The CW EPR spectra for the three samples were fit using the "esfit" function in the EasySpin software package. Each spectrum is labeled with the specific type of taurine that was used when preparing the sample that was analyzed. The ZFS parameters were fixed at D=10 cm<sup>-1</sup> and E/D=0. The additional parameters obtained from fitting the spectra were: Lwpp=3.21 mT and g=[2.023,2.023,2.0059]. The ZFS parameters were fixed and not fit because: 1) the value of ~10 cm<sup>-1</sup> is in line with previously reported values for {FeNO}7 complexes and, at X-Band, any D > ~1 cm<sup>-1</sup> would result in the same spectrum. 2) the sharp, featureless, peak at ~geff=4 suggests a purely axial ZFS (E=0 cm<sup>-1</sup>). Any broadening of the line attributed to a slight deviation from E/D = 0 cannot be measured accurately among the many other potential causes for the broadening.



**Figure S2.** The Fourier transforms of the time domain ESEEM data collected at a field strength of 170 mT prior to taking ratios of the data. Each spectrum is labeled with the specific type of taurine that was used when preparing the sample that was analyzed. The spectra are complex having modulations from couplings to protons, nitrogens, and when present, deuterium nuclei. Additional peaks are noticed in the region of the deuterium Larmor frequency (~1.11 MHz) for the samples prepared with <sup>2</sup>H-taurine but overlap with broad lines from nitrogen couplings (~0.52 MHz) makes direct analysis of this data for deuterium couplings impossible. Analysis of the spectral region where peaks owed to the couplings to protons would be visible (~7.2 MHz) is also hindered by broadened spectral lines



**Figure S3A.** Four pulse HYSCORE spectrum collected at 190 mT field strength for the sample prepared with perdeuterated taurine and the corresponding spectrum for the sample prepared with natural abundance taurine. The spectra show significant overlap in the deuterium Larmor region with 14N cross peaks convoluting the analysis of deuterium cross peaks. Although subtle difference are observed in this region, they are not sufficient for analysis.



**Figure S3B.** Four pulse HYSCORE spectrum collected at 310 mT field strength for the sample prepared with perdeuterated taurine and the corresponding spectrum for the sample prepared with natural abundance taurine. These spectra are subject to the same analysis as Figure S3A.