

## Electronic Structure and Site Dynamics in Copper Doped Tutton Salts

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Temperature dependent Electron Paramagnetic Resonance (EPR) has long been used to evaluate the dynamic Jahn-Teller behavior of copper ions in doped double metal hexahydrate sulfates (Tutton salts). Our recent EPR analysis of doped cadmium creatininium sulfate has expanded these investigations to include metal-organic Tutton salt analogues. The observed range of measured JT and EPR spectral parameters for the  $\text{Cu}^{2+}(\text{H}_2\text{O})_6$  complex in these crystals offers an opportunity to weigh the effect of the host crystal environment on the site dynamics and electronic structure of the copper. To this end, computational chemistry calculations were undertaken for a series of Tutton salts and analogues in order to assess the influence of the host crystalline electric field on the copper unpaired electron wavefunction. DFT computations were performed on clusters centered on the metal-hexaaquo in order to determine atomic charges from which electric field vectors and potentials were deduced at points along the copper-water bonds. Our early analysis shows a much higher electric potential in those Tutton systems which exhibit a more pronounced EPR temperature dependency and hence larger JT dynamic behavior. This reflects a stronger coupling to the lattice in these systems. Also, a rough correlation was found between the unpaired electron  $d_{x^2-y^2}$  orbital spin percentage and the magnitude of the host crystal electric potential. The relationship between the two is being further studied. This work advances our understanding of copper dynamics in biological crystals and how structural and environmental electronic features may facilitate this process.