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Application of EPR studies on Biologically Important Copper Acetyl Acetonate and Copper Tetraphenyl Porphyrin via Bayesian Inference and Density Functional Theory LAXMAN MAINALI, INDRA SAHU, KEITH EARLE, SUNY Albany — Quantitative lineshape analysis can allow one to infer information about spin probe structure and dynamics. Experiments were performed at different frequencies (S, X, K, Q, and W Band) for Copper acetyl acetonate ($Cu(acac)_2$) and 5,10,15,20 - Tetraphenyl - 21H,23H -porphine copper(II) (CuTPP) in toluene at different temperatures. In order to obtain unbiased estimates of model parameters within the context of a given model, EPR spectra were analyzed via methods of Bayesian Inference. Four different sets of model parameters used to describe cw EPR spectra for two different probe symmetries (axial and rhombic) were explored using a model for rotational diffusion that was analyzed via Stochastic Liouville Equation. The optimized magnetic and dynamic tensor parameters were inferred from individual and simultaneous multifrequency fits and were compared with the values obtained from density functional theory (DFT). The isotropic g values estimated with PW1PW for $Cu(acac)_2$ and CuTPP with the respective basis sets 6-31G and 6-31G(d) agree well with the experimental values, whereas the isotropic A values for $Cu(acac)_2$ and CuTPP estimated with Local and gradient corrected functionals PWP and Ahlrichs basis set DZ agree well with the experimental values.

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