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EPR Data Analysis on Copper Complexes using Bayesian Inference, Nonlinear-Least Squares and Statistical Geometry LAXMAN MAINALI, INDRA SAHU, KEITH EARLE, Department of Physics, SUNY Albany — Accurate values of model parameters are required in order to infer information about structure and dynamics from quantitative lineshape analysis. EPR data analysis has been performed on Copper acetylacetonate (Cu $(acac)_2$) and Copper tetraphenyl porphin (CuTPP) using methods of Bayesian Inference, Nonlinear-Least Squares (NLS) and Stastical Geometry. Two site fits for ^{63}Cu and ^{65}Cu have also been successfully performed on Cu $(acac)_2$ using the NLS software package. The static and dynamic parameters for the two site fit have been obtained from Bayesian analysis. The best fit parameters determined by different methods are in agreement. The differential entropy and Channel capacity have been calculated for Cu $(acac)_2$ and CuTPP with and without a Wiener noise filter. The differential entropy was found to be high in both the mixture (^{63}Cu\ ^{65}Cu) and for individual isotopes at W (94GHz) band for Cu $(acac)_2$ and Q (34GHz) for CuTPP. The channel capacity was found to be highest at Q band for both systems which provides a quantifiable metric for the experience of Cu-EPR spectroscopists

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