Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

EPR Spectral Analysis of Vanadyl Model Compounds via Bayesian Inference, Non-linear Least-squares and Statistical Geometry INDRA SAHU, LAXMAN MAINALI, KEITH EARLE, Physics Department, SUNY at Albany — Careful analysis is needed to extract quantitative information from experimental EPR spectra. Spectral analysis has been performed on the model compounds: Vanadyl acetylacetonate (VO $(acac)_2$) and Vanadyl mesotetraphenyl porphin(VOTPP) via methods of Bayesian Inference, Nonlinear Least-squares (NLS) and Statistical Geometry. The magnetic EPR parameters obtained from the Bayesian inference analysis were held fixed, and the dynamic parameters were fitted during the NLS analysis. From that analysis, we found that the best fit parameters are in good agreement in both methods. The differential entropy and Channel capacity have been calculated for the model systems with and without a Wiener noise filter. The differential entropy was found to be highest at W-band (94 GHz) for both model systems. The channel capacity was highest at K-band (23 GHz) for VO $(acac)_2$ and at W-band(94GHz) for VOTPP. We suggest useful experimental design criteria that can be inferred from these observations.

Indra Sahu
Physics Department, SUNY at Albany

Date submitted: 28 Nov 2009 Electronic form version 1.4