

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Multifrequency EPR study of Vanadyl and Copper complexes in the characterization of electron paramagnetic tensor parameters and dynamic parameters** INDRA SAHU, LAXMAN MAINALI, KEITH EARLE, Department of Physics, SUNY at Albany — Vanadyl acetylacetonate, Vanadyl meso-tetraphenylporphine, Cupric acetylacetonate, and Cupric meso-tetraphenylporphine have been studied at S-, X-, K- and Q-band in the rigid limit and in the motional narrowing regime. Data have been analyzed using the Nested Sampling Algorithm developed by J. Skilling based on methods of Bayesian inference. The EasySpin software package is used to simulate the spectral fitting function used in the parameter estimation process. Two different sets of model parameters ( $A_{\parallel}$ ,  $A_{\perp}$ ,  $g_{\parallel}$ ,  $g_{\perp}$ ,  $D_{xy}$ ,  $lw$  and  $A_{iso}$ ,  $\Delta A$ ,  $g_{iso}$ ,  $\Delta g$ ,  $D_{xy}$ ,  $lw$ ) have been used for the data analysis at the various frequencies, both independently and in a simultaneous multifrequency fit. After comparing the results at all the frequencies, it is seen that the magnetic tensor parameters defined from the individual frequency fits fluctuate more among each other in the motional narrowing regime but dynamic parameters do not. The model parameters are better fitted in the case of porphin complexes than that in acac complexes.

Indra Sahu  
Department of Physics, SUNY at Albany

Date submitted: 01 Dec 2007

Electronic form version 1.4