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Application of Bayesian Inference and Relativistic Density Functional Theory on EPR Study of Biologically important Transition Metal (Vanadium) Compounds INDRA SAHU, LAXMAN MAINALI, KEITH EARLE, SUNY Albany — Quantitative lineshape analysis based on the stochastic Liouville equation allows one to infer information about spin probe structure and dynamics. The EPR parameters extracted from Experimental spectra can be used to check theoretical calculation based on Relativistic Density Functional Theory. Experiments on Vanadyl acetylacetonate [$VO(acac)_2$] and Vanadyl mesotetraphenyl porphine [VO(TPP)] in toluene at different temperatures were performed at five different frequencies(S,X,K,Q & W-band). Spectral Analysis was performed using methods of Bayesian Inference at the various frequencies, both independently and in a simultaneous multifrequency fit. Rotational diffusion parameters were inferred for two symmetries (Axial and Rhombic). The isotropic A value (A_{iso}) calculated for $VO(acac)_2$ with unrestricted and hybrid-functional PW1PW and for VO (TPP) with unrestricted and hybrid functional BHLYP and Pople style basis set with polarization function 6-311G(3df,3pd), deviated by 0.95% and 0.23% respectively compared to experimental Aiso values. The isotropic g values (g_{iso}) calculated for VO $(acac)_2$ and VO(TPP) with unrestricted and hybrid-functional PW1PW and Ahlrichs basis set TZV, deviated by 0.18% and 0.05% respectively compared to experimental g_{iso} values.

Indra Sahu
SUNY Albany

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