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Relativistic Density Functional Theory Calculations of the Electron Paramagnetic Resonance Parameters for Vanadyl Acetyl Acetonate and Copper Acetyl Acetonate LAXMAN MAINALI, INDRA SAHU, KEITH EARLE, Department of Physics, SUNY at Albany — Relativistic density functional theory calculations of electron paramagnetic resonance (EPR) parameters using a variety of basis sets have been computed for the model systems Vanadyl acetyl acetonate and Copper acetyl acetonate using the ORCA program. The basis set dependence of g and A tensor calculations for Vanadyl acetyl acetonate and Copper acetyl acetonate were studied using Pople Style and Ahlrichs basis sets in Local and gradient corrected functionals (BP86 and PWP) and Hybrid functionals (B3LYP and PW1PW). The PW1PW hybrid functional gives the best values for $VO(acac)_2$ using the TZV basis set and for $Cu(acac)_2$ using the 6-311G(d) basis set. The calculated A values with PW1PW hybrid functional for $VO(acac)_2$ and Local and gradient corrected functional (BP86) for $Cu(acac)_2$ with same basis set (DZ) give better results than previously reported values using the Amsterdam Density Functional Theory (ADF) Software. Our calculated g and A tensor values are in good agreement with the values determined from experiment.

Indra Sahu
Department of Physics, SUNY at Albany

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