

Detailed Hyperfine Structure of Muoniated Radicals in Planar Phthalocyanines

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Planar phthalocyanines consist of a π -conjugated macrocycle ligand (Pc) with a central cavity where a metallic atom may be bonded. The MuSR signal of these compounds is known from the study of H₂Pc (metal-free phthalocyanine) and ZnPc, where the formation of three distinct muoniated radicals, labeled I, II and III, has been observed [1,2]. Their hyperfine constants were obtained in that work using an isotropic description of the hyperfine interaction [2], but a detailed characterization of the hyperfine structure was recently found to be necessary to understand the spin-dynamics of the states in longitudinal-field geometry.

This work presents the hyperfine structure of states I, II and III in ZnPc extracted from high field TF data considering an axially symmetric description for the hyperfine interaction. It shows that states I and II possess small dipolar parameters with opposite signs, but similar magnitude (Fig. 1), and exhibit a temperature variation consistent with the coupling of the hyperfine interaction to vibrational modes of the outer benzene rings of the molecule. For state III, a large dipolar parameter contrasting with a small isotropic parameter of opposite sign was observed, both bearing a temperature dependence which does not fit any energy expected for the vibrational modes of the rings. This fact, supported by the similarity of hyperfine structure with the Mu_{BC} center, allows proposing an interstitial position for that state which lies between the centers of two stacked phthalocyanine molecules.

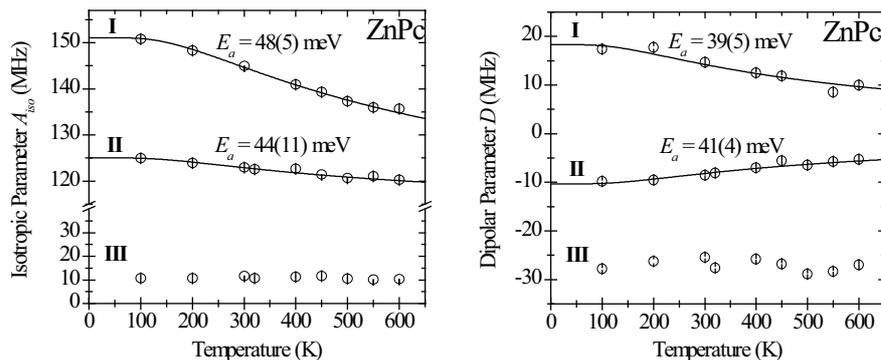


Fig. 1: Temperature dependence of the hyperfine parameters of states I, II and III in ZnPc, as fitted to high transverse field (0.4 T) time spectra.

[1] J. Piroto Duarte et al., Phys. B: Cond. Matt. 326 (2003) 94-96.

[2] J. Piroto Duarte et al., Phys. Rev. B 73 (2006) 075209.