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Magnetic Determination of the Electronic State of Cu and Exchange Interactions in the α- and β-Phases of Molecular Semiconductor Copper Phthalocyanine ($C_{16}H_{32}CuN_8$) ZHENGJUN WANG, KELLY L. PISANE, MOHINDAR S. SEEHRA, Department of Physics and Astronomy, West Virginia University — Among the transition metal phthalocyanines (TMPc, TM = Mn, Fe, Co, Ni, and Cu) in which the TM atoms form linear chains along the b-axis, the electronic structure of CuPc has become of particular recent interest for applications in spintronics [1]. Here, using analysis of magnetization data in the α- and β-phase of powder CuPc samples, the electronic state of Cu and exchange constant are reported. After verifying the crystal structure using x-ray diffraction, the temperature dependence (2 K to 250 K) of the magnetization M of both samples was measured in magnetic field H = 1 kOe and isothermally at 2 K and 5 K in H up to 90 kOe. The data were analyzed first using the modified Curie-Weiss law, $\chi = \chi_o + C / (T+\theta)$, showing good fit for T >4 K and yielding θ = 2.3 K (0.2 K) for α-CuPc (β-CuPc) and spin S = 1/2 characteristic of Cu^{2+}. The data were next fitted to the Bonner-Fisher model for S =1/2 antiferromagnetic Heisenberg chain showing excellent fit to all the M vs. T data and yielding the Cu^{2+}-Cu^{2+} exchange constant J/k_B =3.4 K (0.4 K) the for α-CuPc (β-CuPc). The isothermal data of M vs. H is analyzed taking exchange into account. The large difference in the magnitudes of J/k_B for the two phases is discussed in terms of the differences in their crystal structures [2]. [1] M. Warner et al, Nature, 503, 504-508 (2013). [2] Z. Wang et al, IEEE. Trans. Magn. (in press, Nov. 2015 issue).

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