Abstract Submitted
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Investigation of magnetic structure on $(C_5H_{12}N)CuBr_3$ system on the basis of DFT study and orbital interaction[1] CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang Univ of Sci & Tech, POHANG UNIV OF SCI & TECH TEAM — The $(C_5H_{12}N)CuBr_3$ compound crystallizes in the monoclinic group C2/c. Magnetic susceptibility data down to 1.8 K can be well fitted for the antiferromagnetic spin-1/2 chain, giving the intrachain magnetic coupling constant $J_{intra} \approx -17$ K. At zero field, (pipH)CuBr3 shows 3D order below $T_N = 1.68$ K. Calculated by the mean-field theory, the interchain coupling constant $J_{inter} = -0.91$ K is obtained and the ordered magnetic moment is about 0.23 μ_B. However, the interchain interaction should be strong unlike experimental observation. From the analysis of local structure, the J_{inter} spin dimer show the possibility of good orbital overlap via Cu-O...O-Cu path in which angle for Cu-O...O-Cu is 161° indicating strong interchain interaction via Cu-O...O-Cu path. The magnetic structure of $(C_5H_{12}N)CuBr_3$ system in terms of orbital interaction could anticipated by two-leg spin ladder which such spin ladders interact ferromagnetically to form ladder. In this study, we evaluated spin exchange interactions of $(pipH)CuBr_3$ based on DFT calculations to find the magnetic structure of this system. As a consequence, the J_{inter} interaction is strong and the magnetic structure of this system, indeed, is described by two-leg spin ladder.

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