Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Calculated And Experimental Exchange Interactions In A Strong-rail Spin Ladder; CHRISTOPHER LANDEE, A. SHAPIRO, M. M. TURNBULL, Clark University, Worcester, MA 01610, J. NOVOA, J. RIBAS, Departament de Quimica Fisica, Universitat de Barcelona, Barcelona, Spain. — Low-dimensional magnetic lattices with moderate exchange interactions can be conveniently formed by combining organic cations with tetrahalocuprates. In these compounds, the ultimate structure is ultimately determined by size, shape and hydrogen-bonding capacity of the cation with the magnetic interactions occurring through halide-halide contacts. A variety of these compounds have been studied [1] and techniques have been developed for calculating the magnetic exchange interactions from first principles [2,3]. We report on the synthesis, structure and magnetic properties of (2,3-dimethylpyridinium)$_2$CuBr$_4$, which is the second spin ladder to be found with a stronger rail interactions (J_{rung}/k_B = 9 K, J_{rail}/k_B = 17 K). Comparison will be made between the exchange constants calculated from first principles and those obtained from experimental data. 1. C. P. Landee *et al*, *Phys. Rev. B* **63** 100402 (2001). 2. M. Deumal *et al*, *Polyhedron* **22** 2235-2239 (2003). 3. M. Deumal *et al*, *Euro. J. Inorg. Chem.* **2005**, 4697-4706.

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Date submitted: 07 Dec 2005 Electronic form version 1.4