Abstract Submitted
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Record Two-Halide Exchange in Cu(2,5-dmpz)Br_2: Theory and Experiment R. BUTCHER, C.P. LANDEE, M.M. TURNBULL, Clark University, Worcester, MA 01610, J. NOVOA, J. RIBAS, Departament de Quimica Fisica, Universitat de Barcelona, Barcelona, Spain. — Cu(2,5-dmpz)Br_2 (2,5-dmpz = 2,5-dimethylpyrazine) is an antiferromagnetic rectangular lattice, with the S=1/2 copper ions bridged along one axis through the pyrazine molecules and through Cu-Br. . . Br-Cu contacts in a transverse direction. Large orbital overlap is obtained by the very short Br-Br distances plus the linear arrangement of the copper and bromine atoms. The magnetic susceptibility corresponds to an exchange strength of $J/k_B \approx 160$ K, a record for exchange for two bromide contacts. Numerical techniques have been developed for calculating two-halide contact magnetic exchange interactions from first principles [1,2]. They predict the same exchange strength for Cu(2,5-dmpz)Br_2 based only on the structural parameters of the compound. We present the magneto-structural correlations in Cu(2,5-dimethylpyrazine)Br_2 and compare this to two other known pyrazine complexes; Cu(pyrazine)$CuBr_2$ and Cu(2,3-dimethylpyrazine)Br_2. 1. M. Deumal *et al*, *Polyhedron* **22** 2235-2239 (2003). 2. M. Deumal *et al*, *Euro. J. Inorg. Chem.* **2005**, 4697-4706.

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