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Calculating small interchain exchange parameters in Copper Pyrazine Dinitrate[1] IORWERTH THOMAS, STEWART CLARK, TOM LANCASTER, Durham University — The coordination polymer copper pyrazine dinitrate (Cu(pyz)(NO3)2) is a one-dimensional antiferromagnet that undergoes a magnetic phase transition to a state of long-range three dimensional magnetic order (LRO) below a temperature of 110 mK. The precise nature of the LRO is dependent on the strength of interchain interactions, which are very weak compared to the dominant superexchange interaction along the chain. It is therefore possible that different approaches to ab initio calculations of exchange interaction parameters may be subject to small systematic effects that would lead to erroneous results. In order to investigate whether such a problem arises in this case, we use the GGA+U approach to Density Functional Theory to compare the results obtained by two methods of calculating these parameters: the dimer fragment approach and the periodic method, and relate them to both experiment and previous calculations performed using the hybrid approach.

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