Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Determination of magnetic moments and orbital occupancy in the spin chain compound $Ca_3Co_2O_6$[1] JONATHAN DUFFY, MATTHEW BUTCHERS, University of Warwick, JONATHAN TAYLOR, ISIS, STEPHEN DUGDALE, TOM HAYNES, University of Bristol, STEFANO AGRESTINI, MARTIN LEES, University of Warwick — The one-dimensional cobaltate $Ca_3Co_2O_6$ exhibits a number of intriguing phenomena, including several metamagnetic steps as a function of applied magnetic field. Although it has attracted a considerable amount of research, the origin of the magnetism has not yet been fully determined. We report a measurement of the spin density in $Ca_3Co_2O_6$ using magnetic Compton scattering. The bulk spin moment was determined to be $3.78 \pm 0.05\mu_B$ at 7 T, confirming the existence of a large unquenched Co orbital moment of 1.4 ± 0.1 μ_B. In combination with molecular orbital calculations, the results reveal that double occupation of the $d_{x^2-y^2,xy}$ orbital is responsible for the observed large unquenched orbital moment. Fitting the model to the experimental data shows that there is an induced oxygen moment of 0.8 ± 0.1 μ_B. Unexpectedly, further comparison with KKR-SPA electronic structure calculations strongly indicates the existence of a Fermi surface.

[1]We acknowledge the support of the UK EPSRC via grant EP/F021518.

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Date submitted: 24 Nov 2010 Electronic form version 1.4