Determination of magnetic moments and orbital occupancy in the spin chain compound Ca$_3$Co$_2$O$_6$\textsuperscript{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$_3$Co$_2$O$_6$ 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$_3$Co$_2$O$_6$ 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 $1.4 \pm 0.1 \mu_B$. 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 $0.8 \pm 0.1 \mu_B$. Unexpectedly, further comparison with KKR-SPA electronic structure calculations strongly indicates the existence of a Fermi surface.

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