

## 1PO3-74 Modeling the Specific Heat of the Doped Spin-Chain Compound $\text{Ca}_4\text{Cu}_5\text{O}_{10}$ with Finite Spin-Cluster Behavior

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We report low-temperature specific heat measurements on the highly-doped spin-chain system  $\text{Ca}_4\text{Cu}_5\text{O}_{10}$ . The data can be decomposed into three components: a phonon contribution ( $\sim T^3$ ), a very broad peak near  $T = 25$  K, and a sharper peak near  $T = 13$  K. Since the formal valence of copper is  $\text{Cu}^{2.4}$ , or 0.4 holes per copper ion, a conventional assumption is that 2/5 of the  $\text{CuO}_2$  squares are non-magnetic, most likely due to the formation of Zhang-Rice singlets. We consider the behavior of the 3 remaining magnetically-active Cu ions per formula unit. Susceptibility measurements indicate singlet behavior, suggesting antiferromagnetism or even-number spin clusters. The specific heat data does not indicate long-range order, nor can it be described only by the behavior of isolated dimers. We therefore assumed that while some of the magnetically-active Cu may form isolated dimers, the rest may form other even-number spin clusters. The specific heat of a four-spin cluster was calculated by exact diagonalization in the Heisenberg model. Various configurations, including a four-spin chain segment with intrachain coupling  $J$ , and a cluster of two coupled dimers, with intrachain coupling  $J$  and interchain coupling  $J'$ , were considered. The specific heat of two coupled dimers with ferromagnetic  $J$  and antiferromagnetic  $J'$  most closely resembles the experimental data. We also point out errors in previous four-spin finite-cluster calculations found in the literature.

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