Physics of a new copper-based triangular chain

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Preliminary results

- New cluster compound [(CuCl$_2$\text{tachH})$_3$Cl]Cl, \text{tach} = \text{cis,trans-1,3,5-triamino-cyclohexane} (1,2)

- One-dimensional stack of antiprisms of antiferromagnetically coupled equilateral copper(II) triangles; system is a Heisenberg three-leg ladder with frustrated rung boundary condition.

- Intra-triangle couplings ($J_1$) are drawn by grey lines, inter-triangle couplings ($J_2$) are given by black lines.

(1) Georg Seeber, Paul Kögerler, Benson M. Kariuki, and Leroy Cronin, submitted
• Intra-triangle exchange: bridging chloro ligand and hydrogen bonds; Cu-Cu distance is 4.46 Å.

• Inter-triangle exchange: hydrogen-bonded Cu-Cl⋯H-N-Cu super-exchange; Cu-Cu distance is 6.82 Å.

• Conjecture: weakly coupled triangles, i.e. $|J_2| \ll |J_1|$ $\Rightarrow$ independent triangles at high $T$; effective spin-1/2 chain at low $T$.

(1) Jürgen Schnack, Hiroyuki Nojiri, Paul Kögerler, Geoffrey J. T. Cooper, Leroy Cronin, to be submitted to Phys. Rev. B.
Weakly coupled triangles would result in pronounced plateau at 1/3 of the saturation magnetization.

High-field magnetization measurement show, however, no plateau.

Solution: isotropic Heisenberg model with antiferromagnetic exchange parameters $J_1 = -0.9$ K and $J_2 = -1.95$ K and $g = 2.095$ (average of small $g$-anisotropy).

Deviations at high field: $g$-anisotropy and staggered field; deviations at low field: singlet-triplet gap overestimated in finite systems.
General considerations

- $J_1 = 0, J_2 < 0$: system is bipartite, classical ground state shows collinear Néel order; quantal square lattice on a torus, $S = 0$ non-degenerate (LSM).

- $J_1 < 0, J_2 = 0$: system is three-colorable, classical ground state has coplanar $120^\circ$ order; quantal independent triangles, only two levels, one jump to saturation.

- $J_1 = J_2 < 0$: system is three-colorable, classical ground state has coplanar $120^\circ$ order; quantal triangular lattice on a torus, order?
Zero-temperature properties

- Finite size diagonalizations for [(CuCl$_2$tachH)$_3$Cl]Cl result in a ground state spin $S = 0$.

- Finite size extrapolation with up to 10 triangles shows that the ground state with $S = 0$ is separated from the triplet by $\Delta \approx 0.4 \pm 0.05$ K.
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