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Angaben zur Veröffentlichung / Publication details:

Dumm, M., Martin Dressel, Alois Loidl, and L. K. Montgomery. 1998. "Spin dynamics of organic linear-chain compounds." In *Proceedings of Joint 29th Ampere - 13th ISMAR International Conference, August 2-7, 1998, Berlin, Germany*, 1093-94. Berlin: TU Berlin.

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Spin Dynamics of Organic Linear-Chain Compounds

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Despite two decades of research, the organic charge-transfer salts (TMTCF)₂X ($C = S$ or Se , $X = PF_6$, AsF_6 , ClO_4 , Br , ...) attract considerable interest. The reduced dimensionality leads to instabilities in the electronic system, various ground states like charge-density wave, spin-Peierls, spin-density wave, or superconductivity develop at low temperatures. By slightly changing the organic molecules or the anions, the electronic and magnetic properties can be changed significantly [1].

We carried out electron-spin-resonance experiments in a continuous wave X-band spectrometer on single crystals of (TMTCF)₂PF₆, (TMTCF)₂ClO₄, and (TMTTF)₂Br in the temperature range $1.5 \text{ K} \leq T \leq 500 \text{ K}$ [2]. Here we confine ourselves to results of the spin-chain compounds (TMTTF)₂ClO₄ and (TMTTF)₂PF₆ at $2 \text{ K} \leq T \leq 400 \text{ K}$ (Fig. 1). In the high-temperature regime the spin susceptibility χ_s of both compounds follows the predicted behavior of a $S = 1/2$ antiferromagnetic Heisenberg chain with an exchange constant $J \approx 420 \text{ K}$. The linewidth ΔH is slightly anisotropic and increases almost linear with temperature.

In (TMTTF)₂ClO₄ the ordering of the anions leads to a first-order structural phase transition at $T_{AO} = 72.5 \text{ K}$. This is accompanied by a dimerization of the spin chain leading to a strong decrease of χ_s for $T < T_{AO}$. We determined an alternation parameter $\gamma = 0.83$ and a singlet-triplet gap $\Delta \approx 82 \text{ K}$. At $T \approx 14 \text{ K}$, the ESR signal splits into five lines. It is known from ¹H-NMR experiments that the methyl groups which rotate at high temperatures slow down in this temperature range [3]. Thus the rotational narrowing might be responsible for the hyperfine splitting.

(TMTTF)₂PF₆ undergoes a spin-Peierls transition at $T_{SP} = 19 \text{ K}$. Below T_{SP} , the ESR linewidth ΔH increases and χ_s vanishes exponentially with decreasing temperature. Using mean-field theory, we determined an alternation parameter $\gamma(0) = 0.91$ and a singlet-triplet gap $\Delta(0) \approx 34.5 \text{ K}$. The visible decrease of the spin susceptibility along the b and c direction below $T_{SP}^0 \approx 62 \text{ K}$ can be attributed to 1-D

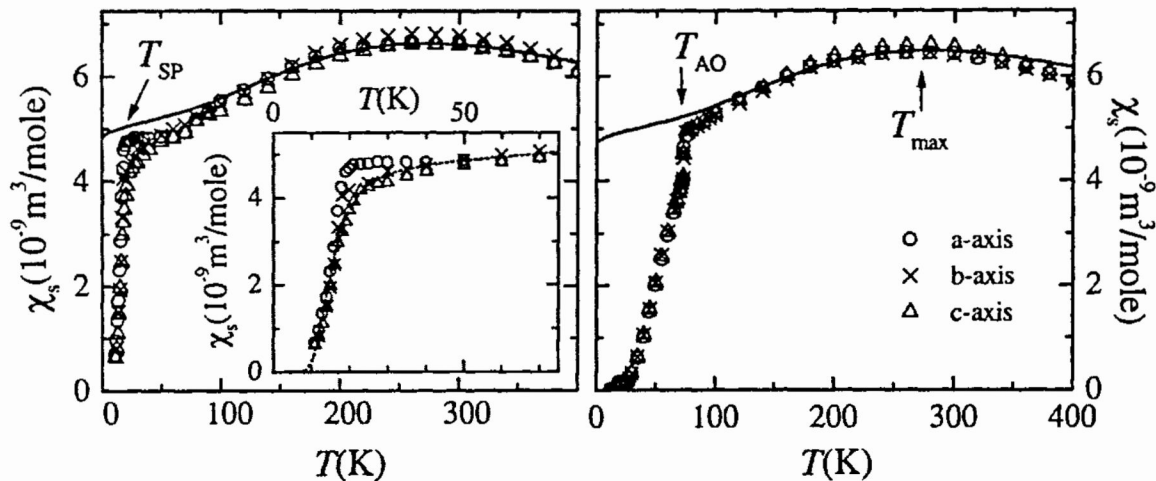


Fig. 1: Temperature dependence of the spin susceptibility χ_s of $(\text{TMTTF})_2\text{PF}_6$ (left) and $(\text{TMTTF})_2\text{ClO}_4$ (right) along the three crystal axes. The solid lines correspond to fits using the EAT-model for a $S=1/2$ AFM Heisenberg chain [4]. The absolute values of χ_s were obtained by scaling the integrated intensity at its maximum value using the relation $\chi_{\text{max}} = C/T_{\text{max}}$, $C = 1.782 \times 10^{-6} \text{ m}^3 \text{ K/mole}$. The inset indicates the fluctuations above the spin-Peierls transition in b and c direction. A good description of χ_s in the SP pseudo-gap regime is given by the dashed line [5].

lattice fluctuations above the spin-Peierls transition [5].

The work at Augsburg was supported by BMBF under contract number EKM 13N6917. The crystal growth at Bloomington was supported by the Division of Material Research of the National Science Foundation (DMR-9414268).

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