

Magnetic Properties of Chain Antiferromagnets RbFeSe₂, TlFeSe₂, and TlFeS₂

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Abstract—Single crystals of ternary ion chalcogenides RbFeSe₂, TlFeSe₂, and TlFeS₂ are studied by X-ray diffraction, SQUID magnetometry, and Mössbauer spectroscopy. Common structural units of these chalcogenides are tetrahedra of FeCh₄ (chalcogen Ch = Se, S), arranged in chains by sharing an edge. It is found that RbFeSe₂, TlFeSe₂, and TlFeS₂ undergo transition to a collinear antiferromagnetic state below temperatures $T_N = 248, 290,$ and 196 K, respectively. Their magnetic moments are oriented perpendicular to the axes of the chains of FeCh₄ tetrahedra.

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INTRODUCTION

The recent discovery of superconductors based on iron [1, 2] has stimulated great interest in studies of iron chalcogenides and pnictides. The main structural feature of iron superconductors is the presence of two-dimensional layers [2, 3] or one-dimensional chains [4] containing tetrahedra of FePn₄ or FeCh₄, where Pn and Ch are pnictogens and chalcogens. The interconnection of superconductivity and structure, and the degree of magnetic moment localization on iron ions, has therefore drawn much attention.

Ternary iron-containing chalcogenides RbFeSe₂, TlFeSe₂, and TlFeS₂ belong to the family of quasi-one-dimensional compounds of the class AFeCh₂ (A = K, Rb, Cs, Tl; Ch = S, Se), in which [FeCh₄] tetrahedra are ordered along crystallographic axis *c* of lattices with shared edges [5–8]. The tetrahedra chains are connected to each other by rubidium or thallium atoms, forming a three-dimensional lattice (see Fig. 1 in [5] and Fig. 9 in [6]) with weak mechanical strength. The minimum distances between iron atoms in the chains (2.83 Å for RbFeSe₂; 2.74 Å for TlFeSe₂; 2.65 Å for TlFeS₂) are close to that of interatomic spacing in metallic iron (2.48 Å) [10]. Such short distances produce strong covalence effects that usually reduce the local spin on magnetic ions and delocalize charge carriers at the Fermi level. This in turn ensures quasi-one-dimensional conductivity along the chains. Ternary iron chalcogenides with AFeCh₂ structure (A =

K, Rb, Cs, Tl; Ch = S, Se) are thus quite interesting and promising objects for investigating the correlation between the structural features of iron chalcogenides and the cooperative phenomena that occur in them (including magnetism and superconductivity).

EXPERIMENTAL

Single crystals of RbFeSe₂, TlFeSe₂, and TlFeS₂ were grown using the Bridgman technique. They had the acicular shape typical for quasi-one-dimensional compounds. Their elemental composition was determined via wavelength-dispersive X-ray microanalysis (WDS EPMA) and showed no deviations from stoichiometry at the 2% level of the measurement error. The phase composition was determined from X-ray diffraction measurements of powder samples at room temperature on a STOE STADI P diffractometer equipped with an X-ray source that had a copper electrode. Rietveld analysis of the diffraction patterns using the FULLPROF software [11] revealed no foreign phases (at least at the sensitivity level of the instrument).

Magnetic measurements were made on a SQUID MPMS5 QUANTUM DESIGN magnetometer in the temperature range of 1.8 to 720 K and magnetic fields of up to 50 kOe. Mössbauer measurements were made on a WissEl constant acceleration spectrometer in the temperature range of 10–300 K; our source of gamma radiation was ⁵⁷Co in a rhodium matrix. The spec-