Incommensurate magnetism in $K_2MnS_{2−x}Se_x$ and prospects for tunable frustration in a triangular lattice of pseudo-1D spin chains

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We report the first detailed investigation of $K_2MnS_2$ and $K_2MnSe_2$ from the $K_2MnS_2$ structure type and their magnetic solid solution $K_2MnS_{2−x}Se_x$ and find that compounds of this structure type consist of strongly-coupled pseudo-one-dimensional antiferromagnetic chains that collectively represent a frustrated two-dimensional triangular antiferromagnet. Bulk samples of $K_2MnS_{2−x}Se_x$ with $0 ≤ x ≤ 2$ are characterized using X-ray diffraction, neutron diffraction, magnetization and heat capacity measurements. An incommensurate cycloid magnetic structure with a magnetic propagation vector $k = [0.58, 0, 1]$ is observed for all samples in $K_2MnS_{2−x}Se_x$, and the ordering is robust despite a 12% increase in cell volume. Geometric frustration of chains results in incommensurability along $a$ and a two-step magnetic transition. The varying geometries accessible in compounds of this structure type are presented as promising avenues to tune frustration.

I. INTRODUCTION

The rich physics in the magnetism of low dimensional and frustrated systems has been a topic of great interest since last 4-5 decades.1, 2 Magnetic frustration, the competition of exchange couplings between localized spins, can be imposed by geometry or competing interactions and has broad implications for ground states and low-temperature properties. At low temperatures, peculiar behavior like spin ices3 and spin liquids2 can result when system fluctuates between different configurations or an ordered frustrated state with noncollinear and/or incommensurate magnetic structures can result with unsatisfied interactions in the Hamiltonian.4, 5

Within such systems, frustration can arise with different dimensionalities. Incommensurate magnetic ordering in quasi-1D magnetic systems can be caused by frustrated intrachain interactions as observed in LiCuVO₄, NaCu₂O₂, and CuCl₂, resulting in magnetic multiferroicity.6−10 or it can be a hallmark of interchain magnetic interactions resulting from frustrated arrangements of chains as observed in triangular-lattice antiferromagnets (TLAFs) such as CsNiCl₃ and Li₂NiW₂O₈.11

In quasi-1D compounds, interchain coupling is required to induce long-range three-dimensional ordering (a Néel temperature) at finite temperatures. Exchange parameters $J_{ij}$ can represent the “ideal” nearest-neighbor (nn) and next nearest-neighbor (nnn) intrachain spin-exchange couplings, here grouped as $J_{\text{intra}}$, while the longer-range interchain coupling between the chains is represented by $J_{\text{inter}}$. (Figure 1) Materials that approach the ideal 1-D Heisenberg limit would be those where the $J_{\text{intra}}$ is strong but $J_{\text{inter}}$ is weak; in this case 3D magnetic ordering may be highly degenerate, incommensurate, or not observed at all.

Identifying systems where exchange interactions are strong but frustrated is therefore of interest, with an additional benefit if the interactions are tunable and a range of spin and geometric constraints could be explored. $K_2MnS_2$ and $K_2MnSe_2$ belong to a rich family of quasi-1D compounds in the eponymous $K_2MnS_2$ structure type, where we concentrate on the representatives where $A_2MX_2$, where $A = K, Na, Rb, Cs; M = Mn, Fe, Co, Zn, Si, Ge, Sn; and X = S, Se, Te, P, As$. $K_2MnS_2$ and $K_2MnSe_2$ were first synthesized by Bronger et al. by the reaction of potassium carbonate with manganese and chalcogen in a stream of hydrogen charged with chalcogen.12 Both these compounds exist in an orthorhombic space group $Ibam$ with edge-sharing $[\text{Mn}_xX_y]^{−6}$ tetrahedral chains along the $c$ direction. Viewed normal to the chains in Figure 1, the chain locations form isosceles triangles with their short distance along (100) and the long distance along (110).

The most closely-related compounds to the $K_2MnS_2$ structure type are the family of $AFeX_2$ ($A = K, Rb, Cs, Tl; X = S, Se$) compounds, which can be divided into three groups based on their crystal and magnetic structures.13 All $AFeX_2$ compounds have tetrahedrally co-
ordinated Fe$^{3+}$ chains along c, but many of these have an additional degree of structural freedom, manifested as a monoclinic distortion (TlFeS$_2$, TlFeSe$_2$, KFeSe$_2$, and RbFeSe$_2$) with the magnetic moments ordered perpendicular to the chains; and KFeS$_2$, RbFeS$_2$ with the ordered moments slightly tilted from the chain axis). [14] [15] Only CsFeS$_2$ is orthorhombic, but it further distorts martensitically at its magnetic transition at 70 K, with moments slightly tilted off the chain direction. [16]

Unlike the well-studied $A$Fe-$X_2$-type compounds, the compounds in the $A_2MX_2$ family have not been examined in sufficient detail to understand any of their magnetic ground states. Only the compound K$_2$CoS$_2$ has been suggested to be a collinear antiferromagnet (on the basis of neutron diffraction by Bronger, but without any published data). [17] The antiferromagnetic nature of K$_2$MnS$_2$ and K$_2$MnSe$_2$ has been suggested based on susceptibility measurements. [12]

In this article, we present an investigation of the magnetic phase diagram of K$_2$MnS$_{2-x}$Se$_x$ using X-ray diffraction, neutron diffraction, magnetization and heat capacity measurements. This is the first detailed study of compounds from the family of $A_2MX_2$-type compounds. We propose an incommensurate antiferromagnetic structure for K$_2$MnS$_2$ using single crystal neutron diffraction and powder neutron diffraction caused by geometric frustration of chains. All compounds in the K$_2$MnS$_{2-x}$Se$_x$ series show similar magnetic ordering and $T_N$, and a two-step magnetic transition characteristic of TLAFs.

II. EXPERIMENTAL PROCEDURE

Bulk synthesis of the samples in the solid solution range of K$_2$MnS$_{2-x}$Se$_x$ with $0 \leq x \leq 2$ in increments of 0.2 was performed out using a solid state tube-in-a-tube method. Handling of reagents was performed in a glove box under argon. Reactions were conducted by loading S and Se in 15 mm diameter quartz tubes in their nominal composition. Metallic K spheres and Mn powder were loaded in a smaller tube resting inside the bigger tube. These tubes were then sealed under vacuum using liquid nitrogen and reacted in box furnaces at 600°C with a ramp rate of 1°C/min and 48 h hold time, followed by furnace cooling. Synthesis of needle-shaped K$_2$MnS$_2$ single crystals was accomplished by high temperature gas flow, similar to the method reported by Bronger. [12] K$_2$CO$_3$ and Mn powder were mixed using a mortar and pestle in a stoichiometric ratio and reacted under an incoming 5% H$_2$/Ar stream charged with S vapor at 757°C.

Powder X-ray diffraction (XRD) measurements were conducted in transmission with a Bruker D8 diffractometer with Mo-K$\alpha$ radiation. Rietveld analysis on X-ray diffraction patterns was carried out using TOPAS 5. [18] All samples were pure as viewed by X-ray analysis except for the $x = 0.2$ sample.

Neutron powder diffraction (NPD) was performed in vanadium cans on the POWGEN instrument at the Spallation Neutron Source at Oak Ridge National Laboratory (ORNL). The temperature was raised from 10K to a maximum of 50K with a ramp rate of 0.5K/min, and longer collections were taken at 10 K and 300 K. Processing and visualization of neutron powder diffraction data was done in the Mantid software. [19]

Single crystal neutron diffraction was collected for K$_2$MnS$_2$ on the HB-3A four-circle diffractometer at the High Flux Isotope Reactor at ORNL, with a neutron wavelength of 1.550 Å selected from a bent perfect Si-220 monochromator. [20] The selected crystal had a size of $0.9 \times 0.2 \times 0.5$ mm and was sealed in a 0.7 mm diameter quartz tube (wall thickness 0.1 mm) to prevent air exposure. The crystal was held in place by another quartz capillary of 0.7 mm diameter. The tube was mounted on the cold head of the closed cycle refrigerator (CCR) to measure the temperature range from 4 K to 450 K. Data were collected at 4.0 K and the (020) and (060) Bragg peaks were measured at increasing temperatures. The nuclear and magnetic structure refinements and representation analysis are carried out with the FullProf Suite. [21] The magnetic symmetry analysis uses the Bilbao Crystallographic Server. [22] [26]

Magnetic susceptibility measurements were collected on a Quantum Design MPMS3 magnetometer. Heat capacity measurements were performed using a Quantum Design Dynacool Physical Property Measurement System (PPMS).
Figure 3. Across the solid solution from K$_2$MnS$_2$ to K$_2$MnSe$_2$, Rietveld refinements to XRD and NPD data show smoothly varying cell volume (a), Se occupancy (a), intrachain Mn–Mn distance (c), and short and long interchain distances (d).

III. RESULTS AND DISCUSSIONS

A. Confirmation of solid solution behavior from X-ray and neutron diffraction

Rietveld refinements to laboratory powder X-ray diffraction show all synthesized compositions K$_2$MnS$_{2-x}$Se$_x$ except the $x = 0.2$ sample (Figure 2). Figure 3 shows the various refined structural parameters variation as a function of $x$ in K$_2$MnS$_{2-x}$Se$_x$ for both laboratory XRD and NPD. The Se occupancy varies linearly with $x$, for both XRD and NPD. Across the whole composition range, increasing the Se content toward K$_2$MnSe$_2$ leads to a 12% volume increase. The difference in ionic radii of S (1.84 Å) and Se (1.98 Å) and increasing covalent nature with $x$ causes an increase in Mn-S/Se bond length. The increase in volume is mirrored by an increase in Mn-Mn distances—both intrachain and interchain as shown in Figure 3 (b) and (c).

Figure 4 (a,b) show the NPD patterns collected at 300 K and 4 K for K$_2$MnS$_{2-x}$Se$_x$. The 4 K data show magnetic peaks for all compositions marked with the pink pointers. The positions and intensities of the peaks provide equivalent magnetic ordering among the samples, but the propagation vector is incommensurate with the nuclear structure.

B. Incommensurate magnetic ordering in K$_2$MnS$_{2-x}$Se$_x$

Magnetic reflections appear below $T = 17$ K for all compositions in K$_2$MnS$_{2-x}$Se$_x$, as shown in Figure 4 (a,b). An order parameter plot for is shown in Figure 5 (c) from single crystal neutron diffraction of K$_2$MnS$_2$. The presence of magnetic reflections in both single crystal and powder neutron diffraction is consistent with our magnetic susceptibility and heat capacity measurements. The mag-
The magnetic phase was indexed using an incommensurate magnetic propagation vector \( k = [0.58 0 1] \) at 4 K. The final refinement of single crystal neutron diffraction data is shown in Figure 6 where the observed and calculated structure factors for the nuclear and magnetic refinements are plotted. The refined magnetic structure results in a cycloidal configuration of magnetic moments in the \( ab \) plane as shown in Figure 7. The spins are antiferromagnetically coupled along the chains in the \( c \) direction. The total refined magnetic moment is 2.279 \( \mu_B \), considerably smaller than 5.92 \( \mu_B \) expected for Mn\(^{2+} \) (\( S = 5/2 \)). A reduced magnetic moment is often observed in quasi-1D spin systems such as NaFeGe\(_2\)O\(_6\), Na\(_2\)TiCl\(_4\) and has been believed to be caused by spin fluctuations and covalency.\(^{29, 30}\) Delocalization of \( d \) electrons could be another explanation for reduced magnetic moment as observed in RbFeSe\(_2\).\(^{13}\) Here, it is more likely that the reduced moment arises from latent disorder due to the frustrated moments in K\(_2\)MnS\(_2\). Accordingly, the steady increase of the magnetic peak (0.42 1 1) order parameter upon cooling to 4 K indicates that the magnetic ordering is not complete.\(^{16}\) Magnetic refinements to the NPD data at 10 K confirm that the cycloid model can be assumed as the magnetic structure for the full substitution range (Figure 5(c)). However, a very good fit for the powder intensity at \( d = 5.23 \) \( \text{Å} \) could not be obtained.

The spin lattice in K\(_2\)MnS\(_2\) and K\(_2\)MnSe\(_2\) is comprised of isosceles triangles, with two nearest-neighbor (\( J_{\text{inter1}} \)) and four next-nearest-neighbor interactions (\( J_{\text{inter2}} \)) as shown in Figure 1(c). The relative strengths of interchain exchange interactions \( J_{\text{inter1}} \) and \( J_{\text{inter2}} \), and \( J_{\text{intra}} \) and anisotropy terms in the Hamiltonian determine the final magnetic ordering of the system. Such a triangular lattice can form a simple non-frustrated square lattice if \( J_{\text{inter1}} = 0 \) and \( J_{\text{inter2}} \neq 0 \), a strongly frustrated triangular lattice if \( J_{\text{inter1}} \approx J_{\text{inter2}} \neq 0 \), and a decoupled spin chain if \( J_{\text{inter1}} \neq 0 \) and \( J_{\text{inter2}} = 0 \). Overall, the netic phase was indexed using an incommensurate magnetic propagation vector \( k = [0.58 0 1] \) at 4 K. The final refinement of single crystal neutron diffraction data is shown in Figure 6 where the observed and calculated structure factors for the nuclear and magnetic refinements are plotted. The refined magnetic structure results in a cycloidal configuration of magnetic moments in the \( ab \) plane as shown in Figure 7. The spins are antiferromagnetically coupled along the chains in the \( c \) direction. The total refined magnetic moment is 2.279 \( \mu_B \), considerably smaller than 5.92 \( \mu_B \) expected for Mn\(^{2+} \) (\( S = 5/2 \)). A reduced magnetic moment is often observed in quasi-1D spin systems such as NaFeGe\(_2\)O\(_6\), Na\(_2\)TiCl\(_4\) and has been believed to be caused by spin fluctuations and covalency.\(^{29, 30}\) Delocalization of \( d \) electrons could be another explanation for reduced magnetic moment as observed in RbFeSe\(_2\).\(^{13}\) Here, it is more likely that the reduced moment arises from latent disorder due to the frustrated moments in K\(_2\)MnS\(_2\). Accordingly, the steady increase of the magnetic peak (0.42 1 1) order parameter upon cooling to 4 K indicates that the magnetic ordering is not complete.\(^{16}\) Magnetic refinements to the NPD data at 10 K confirm that the cycloid model can be assumed as the magnetic structure for the full substitution range (Figure 5(c)). However, a very good fit for the powder intensity at \( d = 5.23 \) \( \text{Å} \) could not be obtained.

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![Figure 5](image-url)  
Figure 5. NPD with increasing T shows disappearance of the magnetic peaks around 15 K for (a) K\(_2\)MnS\(_2\) and (b) K\(_2\)MnSe\(_2\), while triple-axis single-crystal intensity on the (0.4211) peak (c) provides a more precise view of the order parameter evolution. The exact temperature is best judged by heat capacity measurements.

![Figure 6](image-url)  
Figure 6. Calculated vs observed structure factors for nuclear and magnetic reflections obtained from single crystal neutron diffraction refinement of K\(_2\)MnS\(_2\)  

![Figure 7](image-url)  
Figure 7. Magnetic structure of K\(_2\)MnS\(_2\) determined from single crystal neutron diffraction showing the cycloid arrangement of spins in the \( ab \) plane with incommensurability along a direction.
magnetic frustration in K₂MnS₂ manifests itself in the form of incommensurability along a direction. A similar ground state to K₂MnS₂ is seen in the frustrated quasi-1D triangular lattice antiferromagnetic systems CsNiCl₃, CsCoCl₃, NaFeGe₂O₆, and Li₂NiW₂O₈. In the case of Li₂NiW₂O₈, strong anisotropy can overcome the effect of frustration and stabilize a collinear magnetic order. Collinear magnetic structures are also observed in monoclinic compounds, where the unique angle β removes the interchain frustration, as seen in TlFeS₂ and TlFeSe₂.

Comparison of neutron powder diffraction patterns for K₂MnS₂−xSeₓ compounds from Figure 4 reveal similar magnetic ordering in all compositions and the cycloid model is proposed as the magnetic structure in these compounds.

C. Similar Tₙ in K₂MnS₂−xSeₓ

The determination of Tₙ is more precise in these compounds when viewed by magnetic susceptibility, single-crystal neutron diffraction, and heat capacity. Magnetic susceptibility measurements for x = 0.0, 1.0, and 1.8 are displayed in Figure 9. The magnetic susceptibilities of quasi-1D magnets exhibit two characteristic maxima: a broad maximum at high temperatures associated with the short-range intrachain order in 1D, and a sharper kink at low-temperatures associated with the interchain transition into a 3D magnetically ordered phase. The 3D-ordering peak (Tₙ) appears at ~17 K for x = 0, 1, and 1.8. However, our susceptibility measurements up to 300 K do not approach the region of maximum susceptibility due to intrachain coupling, as is typical for related systems with strong 1-D order: KFeS₂ and CsFeS₂ display maxima at T = 565 and 800 K, respectively.

Other compounds, such as TlFeS₂, TlFeSe₂, and RbFeSe₂, show a linear increase in susceptibility above Tₙ and no signs of saturation, which may arise from delocalization of d electrons due to small intrachain Fe-Fe distances. A small degree of itineracy and hence one-dimensional metallic behavior is expected but has never been shown in these ternary iron chalcogenides. Difficulties in handling such fragile, fiber-like crystals and the presence of defects and mechanical breaks in the crystals complicate verification of the metallic nature at a microscopic level. A linear increase in susceptibility has also been observed in two-dimensional metallic layered iron pnictides in the paramagnetic regime, which may arise from the tendency to exhibit moments that have mixed local and itinerant character. The Mn²⁺-Mn²⁺ distance is ~3.1 Å in K₂MnS₂ while the shortest Mn-Mn distance in metallic manganese is 2.67 Å, so some degree of itinerancy can be expected in K₂MnS₂ and K₂MnSe₂.

In the absence of high-temperature susceptibility data showing the broad maximum and paramagnetic behavior following the Curie-Weiss law, existing models for 1D magnetic chains such as the Wagner-Friedberg model, the Rushbrooke-Wood model, the Emori model cannot be used to estimate the value of intrachain coupling as in KFeS₂ and CsFeS₂. If we assume very small degree of itinerancy in K₂MnS₂ and K₂MnSe₂ and that they reach a maximum at higher temperature, results compiled by De Jongh and Miedema can be used to put a lower bound on intrachain coupling constant J using Tₙmax/J ≈ 10.6, giving $J_{\text{intra}} > 28$ K since $T_{\text{max}} > 300$ K. $J_{\text{intra}}$ is governed by the direct and super-exchange interactions between Mn²⁺-Mn²⁺ while $J_{\text{inter}}$, on the other hand, is governed by complicated super-super exchange interactions via Mn–S/Se–S/Se–Mn pathways. While the direct exchange is only governed by distance between...
Mn$^{2+}$-Mn$^{2+}$, the higher levels of exchange interactions depend on two opposing factors: the geometric effect of a larger bridging anion (Se) causing an increase in Mn$^{2+}$-Mn$^{2+}$ distance, and decrease in polarizability of the bridging anion. The final magnetic ordering temperature $T_N$ can be conjectured based on the degree of frustration that arises from the relative strengths of $J_{\text{inter}1}$ versus $J_{\text{inter}2}$, $J_{\text{intra}}$ and anisotropy terms in the Hamiltonian. The balance between these complex terms is surprisingly robust in the case of $K_2\text{MnS}_2-x\text{Se}_x$, since there is no discernible change in $T_N$ across the substitution range.

**E. Interchain anisotropy across many compounds in the $K_2\text{MnS}_2$ structure type**

There are about 30 compounds of the type $A_2MX_2$ in the $Ibam$ $K_2\text{MnS}_2$ structure type reported in the Inorganic Crystal Structure Database. Those with Mn, Co, Fe can be assumed to be magnetic, while others where $M = \text{Zn}, \text{Si}, \text{Ge}, \text{Sn}$ are not. As an arena for tuning magnetic interactions, intrachain couplings can produce systems that are frustrated along one direction, for exam-
pule in LiCuVO$_4$, NaCu$_2$O$_2$, and CuCl$_2$, while separately, these chains interact on a triangular lattice which we show to have much weaker (< 1000 times) interactions. In the K$_2$MnSe$_{2-x}$Se$_x$ system, the triangular lattice is anisotropic, made of isosceles triangles where the long distance is approximately 4% longer than the short distance. In the interest of tuning these distances to further frustrate the system, an ideal triangular lattice would occur when the two distances are equal. At this point we believe that the interchain ordering could be further suppressed, below the ~ 17 K temperatures seen here. In Figure 11, we plot the ratio of the long versus short interchain distance. The only compound that has been examined by neutron diffraction is K$_2$CoSe$_2$, which Bronger and Bomba noted as an antiferromagnet with $T_N$ > 9.5 K, but no data or metrics were included to evaluate the structure solution. Their proposed model included Co moments pointing along the intrachain direction, so there are clearly many degrees of freedom that remain unexplored in this diverse system, and the full list of compounds with distances in ratios is given in Table S1.

IV. SUMMARY AND OUTLOOK

In summary, we have presented the first detailed investigation of K$_2$MnS$_2$ and K$_2$MnSe$_2$ compounds from their eponymous structure type and their magnetic solid solution K$_2$MnS$_{2-x}$Se$_x$. We observe an incommensurate cycloid magnetic structure for all samples in K$_2$MnS$_{2-x}$Se$_x$, identified by single crystal neutron diffraction of K$_2$MnS$_2$ at 4 K and powder neutron diffraction of all samples at 10 and 50 K. The quasi-1D compound is best represented as a 2D triangular antiferromagnet, which results in geometric frustration of chains resulting in incommensurability along a, a two-step magnetic transition characteristic of differing $J_{\text{inter1}}$ and $J_{\text{inter2}}$, and the prospect for tuning these interactions via a wide array of substitution in isostructural compounds.

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