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Antiferro- and metamagnetism in the math

$\text{S}_{\text{m}} = \frac{7}{2} \text{mrow} \text{ hollandite analog math}$

$\text{Eu}_{\text{m}} \text{Ga}_{\text{m}} \text{Sb}_{\text{m}}$

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Antiferro- and Meta-magnetism in the $S=7/2$ Hollandite Analog EuGa_2Sb_2

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Abstract:

Recent work analyzing the impact of non-symmorphic symmetries on electronic states has given rise to the discovery of multiple types of topological matter. Here we report the single crystal synthesis and magnetic properties of EuGa_2Sb_2 , an Eu-based antiferromagnet structurally consisting of pseudo-1D chains of Eu ions related by a non-symmorphic glide plane. We find the onset of antiferromagnetic order at $T_N = 8$ K. Above T_N the magnetic susceptibility is isotropic. Curie-Weiss analysis suggests competing ferromagnetic and antiferromagnetic interactions, with $p_{\text{eff}} = 8.1\mu_B$ as expected for $4f^7 J = S = 7/2$ Eu^{2+} ions. Below T_N and at low applied magnetic fields, an anisotropy develops linearly, reaching $\chi_{\perp}/\chi_{\parallel} = 6$ at $T = 2$ K. There is concomitant metamagnetic behavior along χ_{\parallel} , with a magnetic field of $\mu_0 H \approx 0.5$ T sufficient to suppress the anisotropy. Independent of crystal orientation, there is a continuous evolution to a field polarized paramagnetic state with $M = 7\mu_B/\text{Eu}^{2+}$ at $\mu_0 H = 2$ T as $T \rightarrow 0$ K. Specific heat measurements show a recovered magnetic entropy of $\Delta S_{\text{mag}} \approx 16.4 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ from $T \sim 0$ K to $T = T_N$, close to the expected value of $R\ln(8)$ for an $S = 7/2$ ion, indicating negligible low dimensional spin fluctuations above T_N . We find no evidence of unusual behaviors arising either from the dimensionality or the presence of the non-symmorphic symmetries.

I. Introduction:

Zintl phase compounds have earned a lot of recognition due to their polyanionic and cationic networks in areas of thermoelectric, topological materials, and magnetic materials.¹⁻¹⁰ The structural motifs offered by Zintl phase materials are quite appealing due to the electrostatic interactions between cations and anions and covalent interactions in the polyanionic framework. This setting causes the materials to often behave as two independent subunits, with separate magnetic and electronic behaviors from the cations and polyanionic framework if the cations are magnetic and the anions are non-magnetic.

When the cation is magnetic, the interplay between magnetism and structure could yield versatile ground states. Rare earth based Zintl materials is extensively studied in terms of electronic transport. However, their magnetic structures have scarcely been studied.¹¹⁻¹⁵

Similarly, recent work has demonstrated how non-symmorphic symmetries can conspire to generate unique topological electronic states of matter, such as Dirac 6-fold and 8-fold fermions, as well as more general topological states such as those found in $\text{GdSb}_x\text{Te}_{2-x-\delta}$, CeSbTe , and GdSbTe .¹⁶⁻²²

The magnetic Zintl phase EuGa_2Sb_2 was recently reported to exist based on a

polycrystalline synthesis.²³ The reported crystal structure from single crystal X-ray diffraction^{24,25} has space group $Pnma$ and has non-symmorphic symmetries that relate to adjacent magnetic ions. Further, electron counting implies divalent Eu^{2+} , which has a half-filled f-shell ($4f^7$) and $L=0$, which considerably simplifies the interpretation of magnetic behavior^{24,25}. Thus, EuGa_2Sb_2 provides an opportunity to explore the effects of non-symmorphic symmetries on magnetic order.

This work reports the synthesis of single crystals of EuGa_2Sb_2 via flux growth, confirms the crystal structure by single crystal X-ray diffraction and studies the magnetic properties via magnetization and specific heat measurements. The crystal structure is describable as an analog of Hollandite, with a Ga_2Sb_2 framework forming 1D channels in which Eu ions form pseudo-1D chains. We find the onset of antiferromagnetic order at $T_N = 8$ K, consistent with Mössbauer experiments²⁴. Above T_N , Curie-Weiss analysis yields $p_{\text{eff}} = 8.1\mu_B$ as expected for $4f^7 J = S = 7/2$ Eu^{2+} ions. A positive Weiss temperature $\theta = 5.89$ K suggests competing ferromagnetic and antiferromagnetic interactions. The magnetic susceptibility is direction-independent above T_N , with an anisotropy developing linearly below T_N , reaching $\chi_{\perp}/\chi_{\parallel} = 6$ at $T = 2$ K. There is concomitant metamagnetic behavior along χ_{\parallel} , with a magnetic field of $\mu_0 H \approx 0.5$ T sufficient to suppress the anisotropy. There is also a continuous evolution to a field polarized paramagnetic state with $M = 7\mu_B/\text{Eu}^{2+}$ at $\mu_0 H = 2$ T as $T \rightarrow 0$ K. Specific heat measurements show a sharp transition at T_N , with a broad tail of entropy loss at lower temperatures. The estimated recovered magnetic entropy of $\Delta S_{\text{mag}} = 16.4 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ from $T \sim 0$ K to $T = T_N$ is close to the expected value of $R\ln(8)$ for an $S = 7/2$ ion. This behavior indicates little low dimensional spin fluctuations above T_N , despite the low dimensionality implied by the crystal structure, and attributed to the large value of S .

Together; these results allow us to gain insights into the nature of magnetism in Eu-based Zintl compounds and its correlation to the structure and thermodynamics quantities.

II. Methods:

A. Experimental:

Single crystals of EuGa_2Sb_2 were synthesized from Eu (ingot, Yeemeida Technology Co., LTD 99.995%), Ga (ingot, Noah Tech 99.99%), and Sb (BTC, 99.999%) using the binary flux technique. The elements were put in Canfield crucibles (size: 2mL) in 50:110:150 ratio for Eu:Ga:Sb with a total composition mass of 5 grams. Ga and Sb were placed in the crucible at atmospheric conditions, while Eu was added last in an Ar-filled glove box. The Canfield crucible was placed in a quartz ampoule with quartz wool below and above the crucible, evacuated, and sealed under 1.2×10^{-2} torr of pressure.²⁶ The evacuated ampoules were loaded in a box furnace at an angle of 45° . The temperature was ramped at $80^\circ\text{C}/\text{h}$ to $T=550^\circ\text{C}$ for 12 hours. This step allows for Ga and Sb binary flux to be in a liquid state. The furnace was then ramped from $T=550^\circ\text{C}$ to $T=1100^\circ\text{C}$ at the rate of $80^\circ\text{C}/\text{h}$ and held for 24 hr. The furnace was then slowly cooled to $T=650^\circ\text{C}$ at the rate of $5^\circ\text{C}/\text{h}$, then removed hot, inverted, and immediately centrifuged. Centrifugation took 2-3 minutes. Rod shaped crystals of size 1-1.5 mm along the long direction were removed from the frit. These single crystals of EuGa_2Sb_2 were found to be stable on the benchtop.

Powder X-ray diffraction (XRD) patterns were collected over an angle range of $5\text{-}60^\circ$ on a laboratory Bruker D8 Venture Focus diffractometer that utilizes a LynxEye detector and $\text{Cu K}\alpha$ radiation. Structural refinements were performed with GSAS-II, and resulting structures were visualized with Vesta software.²⁷ Single crystal X-ray data were collected on a Bruker-Nonius X8 Proteum ($\text{Mo K}\alpha$ radiation)

diffractometer. SADABS was used to apply the absorption correction using the ‘multi-scan’ approach.²⁷ All calculations were performed using the SHELX software package. The structures were solved by direct methods, and successive interpretations of difference Fourier maps were followed by least-squares refinement.^{28,29}

Magnetization data were collected on a Quantum Design Magnetic Property Measurement System (MPMS). Magnetic susceptibility was approximated as magnetization divided by the applied magnetic field ($\chi \approx M/H$). In addition, heat capacity data were collected on a Quantum Design Physical Properties Measurement System using the semi-adiabatic method and a 1% temperature rise.

III. Result and Discussion:

A. Structure

Powder XRD scans of EuGa_2Sb_2 were consistent with the previously reported structure in space group Pnma (62). The as grown single crystals of EuGa_2Sb_2 showed phase purity via powder refinement. The results of single crystal diffraction data refinements, tables 1 and 2, are consistent with the prior literature reports from powder diffraction refinements. **The as grown single crystals, is shown in Figure 1(a) and a precision image from single crystal refinement image is shown in Figure 1(b).** From an electron counting perspective, the compound is expected to be built of Eu^{2+} cations, and a $[\text{Ga}_2\text{Sb}_2]^{2-}$ anionic Zintl framework, and that is indeed the case. **Figure 1(c)** shows that the structure is built of $[\text{Ga}_2\text{Sb}_2]^{2-}$ units that form structural motifs of tetrahedral and bridging Sb in a square-chain ladder format.²³⁻²⁵ The squares consist of 2 bridging Sb and 2 Ga atoms, and the ladder consisting of Ga-Ga chains. These form an extended network with one-dimensional channels in which Eu^{2+} ions reside.

The EuGa_2Sb_2 structure is comparable to EuLu_2Se_4 and $\text{K}_2\text{Sn}_3\text{O}_7$, crystallizing in the Pnma space group and analogous to the Hollandite structure type.^{30,31} **In Figure-1(d) and (e),** we see the classic $\alpha\text{-MnO}_2$ structure type of Hollandite in EuLu_2Se_4 and $\text{K}_2\text{Sn}_3\text{O}_7$. In these structures, there is a presence of 1D chains with the cations Eu^{2+} and K^+ ions spaced $4.0470(4) \text{ \AA}$ and $3.12250(9) \text{ \AA}$ apart, respectively, within each chain. In comparison, the structure of EuGa_2Sb_2 is an analog with Eu^{2+} as the cation forming chains with a spacing of $4.3225(8) \text{ \AA}$. One difference is that the anion chains of $[\text{Ga}_2\text{Sb}_2]^{2-}$ form smaller networks of tetrahedral and bridging Sb in a square-chain ladder format instead of face sharing octahedral in the other two structures. This pseudo-Hollandite structure in EuGa_2Sb_2 is also structurally distinct from other pseudo-Hollandite structures such as PbIr_4Se_8 and TiCr_5Se_8 occupancy of the 1D chains with transition metals and charge balancing of Ti^{1+} and Cr^{3+} .^{32,33} In all cases there are non-symmorphic glide plane symmetries present that relate Eu^{2+} ions in adjacent channels.

B. Heat capacity

Temperature-dependent heat capacity measurements were carried out to understand the magnetic contribution of Eu and phononic contribution in the EuGa_2Sb_2 single crystals. Figure 2 shows the heat capacity as a function of temperature in EuGa_2Sb_2 from 2-225 K. The heat capacity plot showed a sharp phase transition at $T = 7.4 \text{ K}$. At $T = 225 \text{ K}$, the Dulong-Petit limit was observed. This limit is calculated using the $C_p = 3NR$, where N is the number of atoms and R is the ideal gas constant.³⁴ In EuGa_2Sb_2 , the number of atoms is 5, and the value is approximately equal to $124 \text{ J mol}^{-1} \text{ K}^{-1}$ respectively. In order to generate the change in entropy from the magnetic order, the phonons were subtracted by modeling the high temperature specific heat using a two Debye phonon model and then removing that as the

phonon contribution at all temperatures. The two Debye model is:

$$\frac{C_p}{T} = \frac{C_D(\theta_{D1}, s_1, T)}{T} + \frac{C_D(\theta_{D2}, s_2, T)}{T} \quad (1)$$

$$C_D(\theta_D, T) = 9sR \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{(\theta/T)^4 e^{\theta/T}}{[e^{\theta/T} - 1]^2} d\frac{\theta}{T} \quad (2)$$

Where θ_{D1} and θ_{D2} are the Debye temperatures, s_1 and s_2 are the oscillator strengths, and R is the molar Boltzmann constant. The model parameters from the least-squares refinement to the data for $T > 16$ K, Figure 3(a), are given in Table 3. The total oscillator strength $s_1 + s_2 = 5.2(2)$. This is in good agreement with the expected value of $1+2+2 = 5$, the total number of atoms per formula unit in EuGa_2Sb_2 .

After subtracting this phonon contribution, the sample heat capacity from $T=2$ - 225 K was integrated to determine the change in entropy corresponding to magnetic order in EuGa_2Sb_2 . Figure 3(b) shows that the change in the magnetic entropy reaches a maximum of $\Delta S_{mag} \approx 16.4 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$, close to the $R\ln(8) = 17.2 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ expected for an $S=7/2$ system. The small discrepancy is attributable to the use of a linear extrapolation to capture the entropy from $T = 0$ to 2 K. The recovery of a full $R\ln(8)$ entropy is not unexpected, being seen in many divalent (Eu^{2+}) materials such as EuMg_2Bi_2 and $\text{Eu}_3\text{In}_2\text{P}_4$. This behavior contrasts to mixed valent (Eu^{2+} and Eu^{3+}) compounds such as EuZnSb_2 and EuIr_2In_8 and supports our assignment of Eu^{2+} on crystal-chemical grounds.³⁵⁻³⁸ Further, recovery of the full $R\ln(8)$ indicates minimal splitting of states due to crystal field effects. This effect arises from the fact that $L=0$ and that the local point symmetry of each Eu^{2+} ion is C_m : by symmetry, the ground state $^8S_{j=7/2}$ is allowed to split into four doublets, and the entropy from all four of these doublets must be recovered to reach $R\ln(8)$. However, the existence of these doublets may explain why the transition observed in specific heat is not a single sharp anomaly but instead has a pronounced tail extended well below the transition temperature. Third, more than 90% of the entropy is recovered

below T_N . This trend indicates negligible loss of entropy above T_N , and implies a lack of low dimensional but longer range magnetic correlations. **It is also important to note that in the case of Eu^{2+} , the next excited state is present at high energy that Schottky anomalies by magnetic excited state may be safely excluded as a possibility over the measurement range.**³⁹ Despite the structure being built of pseudo-1D chains, the physical behavior does not have a regime in which the expected 1D physics is dominant; this might be due to the large S , which is known to suppress fluctuations.

C. Magnetization

To further elucidate the magnetic properties of EuGa_2Sb_2 , magnetization as a function of temperature and field were studied. The $M(T)$ plots in Figure 4(a) and (b) show an evident antiferromagnetic phase transition at $T_N=8.3$ K and $T_N=7.9$ K in the parallel and perpendicular direction to the b axis, respectively. To further quantify the magnetic susceptibility results, the high temperature, $T=50$ - 300 K data were fitted to the Curie-Weiss law:

$$\chi = \frac{C}{T - \theta_{cw}} \quad (3)$$

Here C is the Curie constant, and θ_{cw} is the Weiss temperature. The fit is shown in Figure-4(d) and 4(e), respectively. The p_{eff} extracted from the Curie constants are 8.16 and 8.15, respectively, close to the theoretical p_{eff} for Eu^{2+} , in agreement with expectations and the specific heat results. Thus, the positive Weiss constants indicate dominant ferromagnetic interactions; in combination with the observed antiferromagnetic order, this indicates substantial antiferromagnetic and ferromagnetic interactions.

The M/H behavior is found to vary with the strength of the applied magnetic fields. The field dependence on $M(T)$ shows a decrease in the ordering temperature with increasing field at low temperatures, becoming field independent beyond $T=40$ K in both directions. Another

observation was that in $\mu_0 H \perp b$, the $\mu_0 H = 0.5\text{-}2\text{T}$ range had the same magnitude in magnetization at $T = 2\text{K}$. However, the $\mu_0 H // b$ showed a monotonic decrease. These observations indicate the presence of anisotropy at low temperatures. Figure 4(f) shows the magnetization ratio in the parallel and perpendicular directions; above T_N , the ratio is 1, indicating no anisotropy. Below T_N , the anisotropy rises linearly, reaching a value of 6 at $T = 2\text{K}$.

To further investigate the effect of anisotropy between the $\mu_0 H // b$ and $\mu_0 H \perp b$ in EuGa_2Sb_2 single crystals, magnetization as a function of the magnetic field was studied. Figure 5 (a) and (b) show that the effective moment reaches the theoretical saturation for Eu^{2+} in parallel and perpendicular directions along the b plane at high fields, indicative of a field-polarized state. This result further confirms the assignment of Eu valence as Eu^{2+} . Further, the shapes of the $M(H)$ curves are different between the two directions below T_N , consistent with the observed appearance of anisotropy.

The measurements with $\mu_0 H // b$ show a metamagnetic transition seen at temperatures below the ordering temperature at $\mu_0 H = 0.5\text{T}$, as seen in Figure 5 (a) inset. Metamagnetism is seen in most Co and Eu compounds because of single-ion anisotropy, but not expected here due to the isotropic nature of a $4f^7$ ($S=7/2$) state.^{40,41} Instead, we attribute this metamagnetism as a consequence of the magnetic order, which fixes the spins relative to each other, making some directions more easily polarizable than others. These behaviors can be further observed in the derivatives: Figure 5 (c) and (d) show the change in derivative as a function of the field from the $M(H)$ plots, which further illustrate the metamagnetic transitions in $\mu_0 H // b$ below T_N ; while $\mu_0 H \perp b$ has a monotonic trend. In general, these magnetism trends explain that the $\mu_0 H // b$ shows a lower induced magnetization at low applied magnetic fields. It is thus considered the hard axis (from the perspective of local spins) for

ferromagnetic orders, and the easy axis in the case of antiferromagnetic order.⁴²

Combining these results yields the magnetic phase diagrams shown in Figure 6(a) and (b). Below $\sim 0.5\text{T}$, the system is in an antiferromagnetic state in which the applied field is not sufficient to overcome the anisotropy. Between ~ 0.5 and $\sim 2\text{T}$, the spins reorient following the applied field and develop increasing (magnetic) polarization until, finally, a field-polarized ferromagnetic/paramagnetic state is reached.

From these results, we can speculate on the type of magnetic order that is present. First, the material is antiferromagnetic; this necessitates antiferromagnetic order along at least one crystal direction. Second, the positive Weiss constant suggests ferromagnetic order along at least one direction. This result leaves three possible general states, shown in Figure-6 (c,d,e): ferromagnetic chains with alternating (c) or block (d) antiferromagnetic order between chains, or (e) antiferromagnetic chains with ferromagnetic order between chains. Finally, the direction of the magnetic moments is only loosely constrained: from the previous discussion in the $M(H)$ plots, it is clear that $\mu_0 H // b$ has smaller induced magnetization at low fields, but that can be explained either by spins that lie parallel to a with antiferromagnetic order perpendicular or by spins perpendicular to a but with ferromagnetic order parallel. Future neutron studies, challenging due to the highly absorbing nature of Eu, would be needed to discriminate between these possibilities.

IV. Conclusion:

The structure of EuGa_2Sb_2 crystallizes in the space group Pnma (62).²³⁻²⁵ The single crystals are synthesized for the first time using the flux technique. The EuGa_2Sb_2 structure is characterized to be a Hollandite analog and thus having pseudo-1D chains. The change in magnetic entropy recovered reaches the

theoretical limit of $R\ln(8)$ for Eu^{2+} ions, implying no frustration or fluctuations above T_N , and a small splitting in the crystal field levels. The magnetic properties reveal that EuGa_2Sb_2 is anisotropic below T_N , and has a metamagnetic transition along $\mu_0 H // b$. The magnetic phase diagram reveals the two magnetic phases in the structure and three possibilities in the magnetic structure. Overall, our results help us gain insights into the structure and magnetism in EuGa_2Sb_2 . For future work, neutron diffraction could further help elucidate the magnetic structure, and determine whether nonsymmorphic symmetries have any impact on the magnetic excitations that are present.

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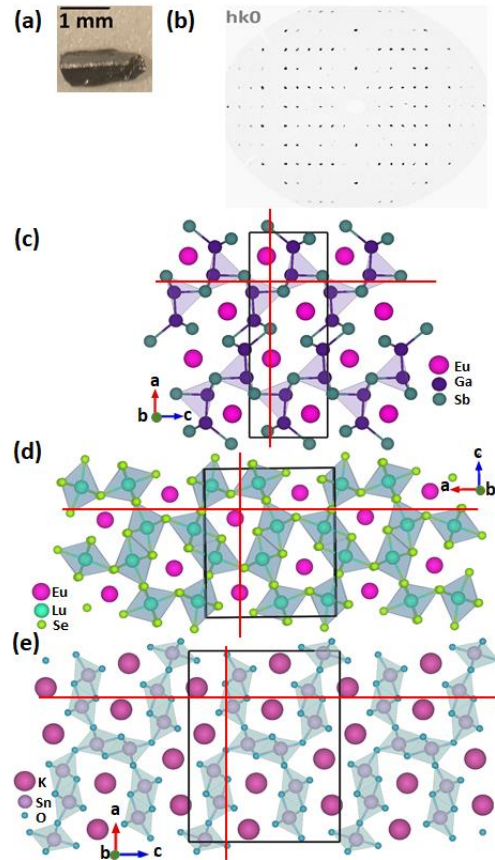


Figure-1 (a) As grown single crystal image of EuGa_2Sb_2 , (b) Single crystal precision image of $(hk0)$ plane. Structures of (c) EuGa_2Sb_2 ,²³⁻²⁵ (d) EuLu_2Se_4 ,³⁰ and (e) $\text{K}_2\text{Sn}_3\text{O}_7$ ³¹ that crystallize in Pnma and are Hollandite-like structures containing 1D chains of ions in channels; red lines indicate the non-symmorphic glide planes. The black box represents a unit cell single crystal X-ray diffraction.

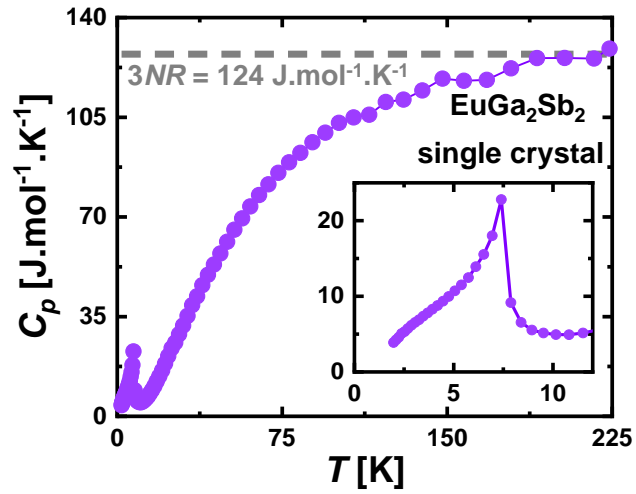


Figure-2 Temperature-dependent heat capacity of EuGa_2Sb_2 single crystals at $\mu_0H=0.1\text{T}$ from $T=2\text{-}225\text{K}$. The sharp transition at $T=7\text{K}$ is attributed to the antiferromagnetic phase transition. The Dulong-Petit theoretical value of $3NR=124\text{ J.mol}^{-1}.\text{K}^{-1}$ is reached around $T = 200\text{ K}$. **The inset shows the magnified antiferromagnetic phase transition at $T=7\text{K}$.**

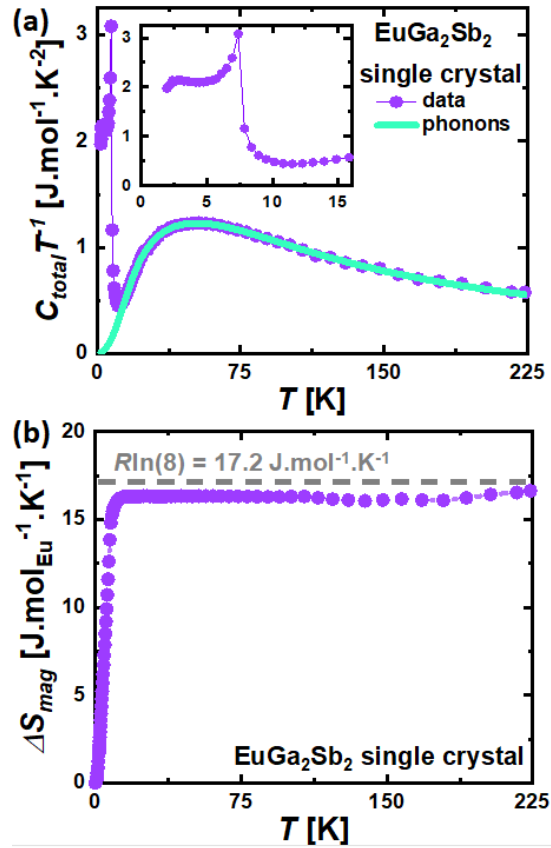


Figure-3 (a) Heat capacity divided by temperature as a function of temperature for EuGa₂Sb₂ single crystals at $\mu_0 H = 0.1$ T from $T = 2$ -225 K. The purple are the data points, and the aqua is the phonons modeled using the two Debye models from $T = 16$ -225 K. The sharp transition at $T = 7$ K is attributed to the antiferromagnetic phase transition. (b) The change in magnetic entropy was integrated after subtracting the phonons from 2-225 K. The ΔS_{mag} is close to the $R \ln(8)$ expected for an $L = S = 7/2$ system.

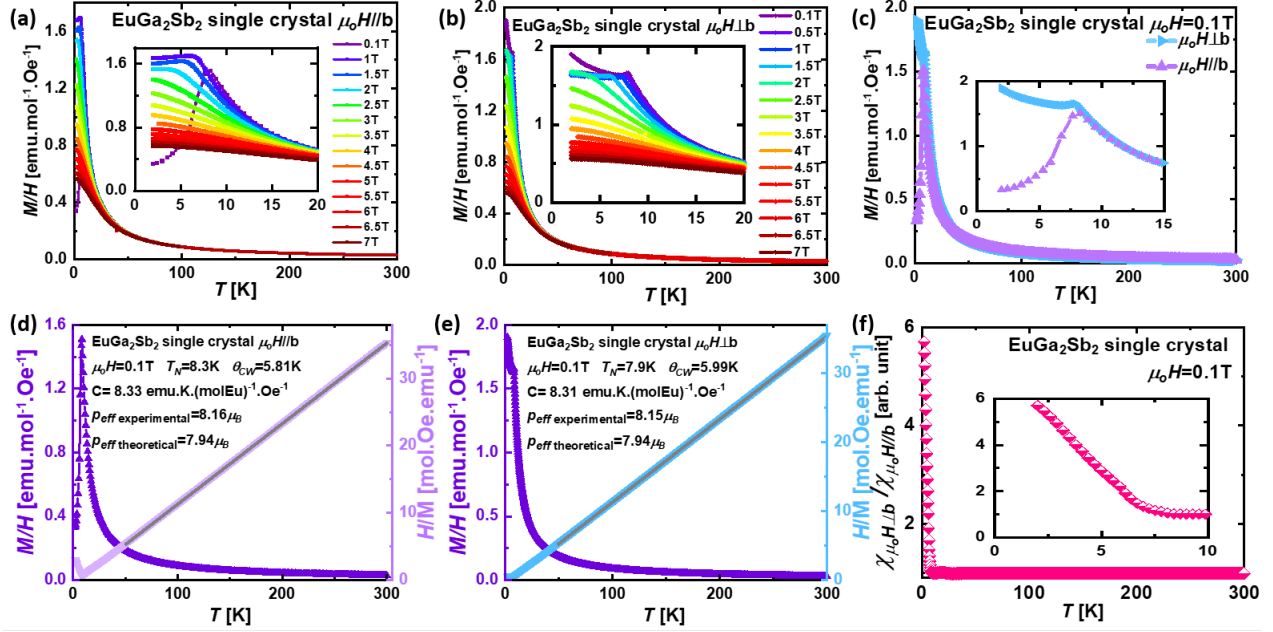


Figure-4 (a) Magnetization as a function of temperature with $\mu_0 H // b$ and $\mu_0 H = 0.1-7$ T and $T=2-300$ K. The $\mu_0 H = 0.1$ T data shows a clear AFM transition at $T = 7$ K, with a decrease in both sharpness of the transition and the temperature of the transition as the field increases. (b) Magnetization as a function of temperature $\mu_0 H \perp b$ from $\mu_0 H = 0.1-7$ T and $T=2-300$ K. The $\mu_0 H = 0.1$ T data shows a kink at $T = 7$ K followed by an upturn, both of which are suppressed for $\mu_0 H > 0.1$ T. (c) Comparison in the magnetization as a function of temperature, $\mu_0 H \perp b$ and $\mu_0 H // b$, at $\mu_0 H = 0.1$ T over $T=2-300$ K, (d) Curie Weiss analysis for $\mu_0 H // b$ from $\mu_0 H = 0.1$ in the range $T=2-300$ K, (e) Curie Weiss analysis $\mu_0 H \perp b$ from $\mu_0 H = 0.1$ and $T=2-300$ K, and (f) Ratio of magnetization $\mu_0 H // b$ and $\mu_0 H \perp b$ at $\mu_0 H = 0.1$ T and $T=2-300$ K displaying the anisotropy below T_N .

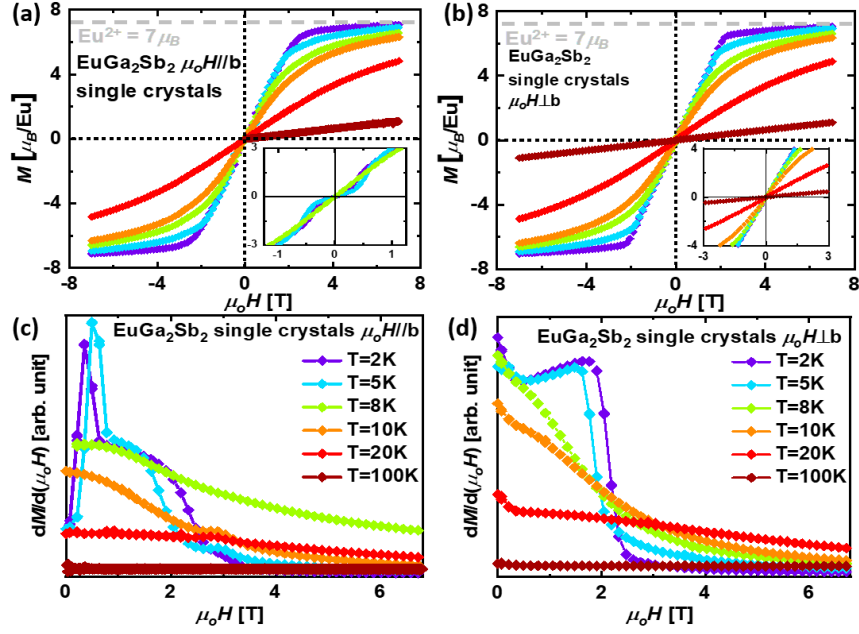


Figure-5 (a) Magnetization as a function of magnetic field with $\mu_0 H // b$ from $\mu_0 H = -7$ to 7T and $T=2, 5, 8, 10, 20,$ and 100 K. (b) Magnetization as a function of magnetic field with $\mu_0 H \perp b$ from $\mu_0 H = -7$ to 7T and $T=2, 5, 8, 10, 20,$ and 100 K, (c) derivative of magnetization over magnetic field as a function of magnetic field with $\mu_0 H // b$ at $T=2, 5, 8, 10, 20,$ and 100 K, and (d) derivative of magnetization over magnetic field as a function of magnetic field with $\mu_0 H \perp b$ at $T=2, 5, 8, 10, 20,$ and 100 K. There is a clear metamagnetic behavior below ~ 0.5 T.

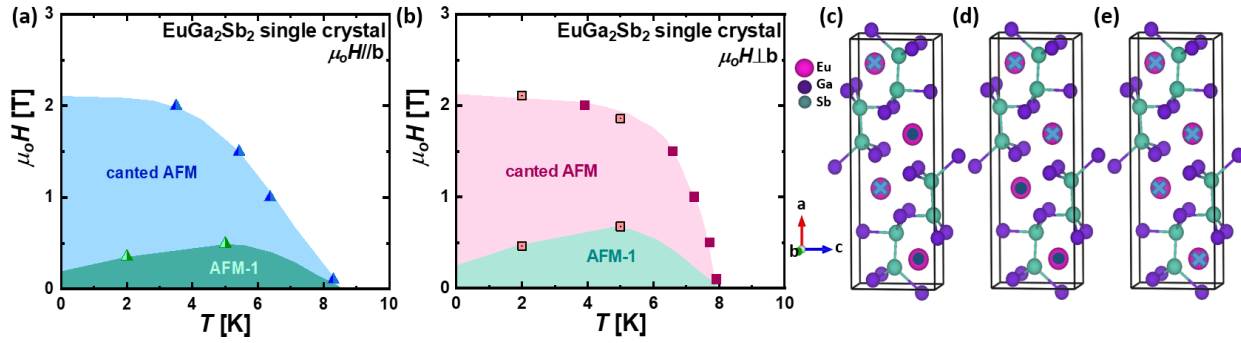


Figure-6 (a) Magnetic phase diagram of EuGa₂Sb₂ with $\mu_0 H // b$. (b) Magnetic phase diagram of EuGa₂Sb₂ with $\mu_0 H \perp b$. In both cases, there is an anisotropic AFM state at low fields, followed by a canted AFM state that continuously evolves to a field polarized state. The transition from AFM-1 to canted AFM was determined from the first maximum (minimum) in the $M(H)$ derivative data for $\mu_0 H // b$ and $\mu_0 H \perp b$ respectively. The transition from canted AFM to a field polarized state was determined from the maximum in the $M(T)$ data. (c,d,e) Possible magnetic structures for EuGa₂Sb₂. In (c,d), the chains are ferromagnetic along the chain direction (into the page), while in (e) the chains are antiferromagnetic along the chain direction. The light blue x represents spin up, while the dark blue o represents spin down.

Formula	EuGa ₂ Sb ₂
Crystal system	Orthorhombic
Space Group	<i>Pnma</i> (No. 62)
a (Å)	18.2201(4)
b (Å)	4.2987(1)
c (Å)	6.6994(1)
V (Å ³)	524.715(19)
Z	4
M/gmol ⁻¹	534.93
ρ ₀ /gcm ⁻³	6.772
μ/mm ⁻¹	31.895
Radiation	Mo Kα, λ= 0.71073 Å
Temperature (K)	90 K
Reflections	1481/86
collected/number of parameters	
Goodness-of-fit	1.373
R[F] ^a	0.0207
R _w (F _o ²) ^b	0.00510

$$^a \mathbf{R}(\mathbf{F}) = \frac{\sum ||\mathbf{F}_o| - |\mathbf{F}_c||}{\sum |\mathbf{F}_o|}$$

$$^b \mathbf{R}_w(\mathbf{F}_o^2) = [\sum w(\mathbf{F}_o^2 - \mathbf{F}_c^2)^2 / \sum w(\mathbf{F}_o^2)^2]^{1/2}$$

	Occ.	Wyckoff Positions	x (Å)	y (Å)	z (Å)	U _{eq} (Å ²)
Eu	1	4c	0.3847(1)	0.7500	0.7802(1)	0.003(1)
Ga1	1	4c	0.4293(1)	0.2500	0.4418(1)	0.004(1)
Ga2	1	4c	0.2921(1)	0.2500	0.4636(1)	0.004(1)
Sb1	1	4c	0.2872(1)	0.2500	0.0640(1)	0.003(1)
Sb2	1	4c	0.4694(1)	-0.2500	0.2315(1)	0.003(1)

	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Eu	0.00349	0.00349	0.00325	0	0.00002	0
Ga1	0.00416	0.00369	0.00444	0	0.00001	0
Ga2	0.00381	0.00367	0.00343	0	0.00001	0
Sb1	0.00278	0.00282	0.00269	0	0.00015	0
Sb2	0.00347	0.00321	0.00351	0	-0.00026	0

Table 1. Crystallographic parameters of the SXRD for EuGa₂Sb₂.

s_{D1} (oscillator strength/formula unit)	s_{D2} (oscillator strength/formula unit)	θ_{D1} (K)	θ_{D2} (K)
3.2(2)	2.05(9)	293(15)	121(2)

Table 2. Fitting parameters to the C_p/T as a function of T for EuGa_2Sb_2 to extract the phonon contribution.

EuGa_2Sb_2	$\mu_0 H // \mathbf{b}$	$\mu_0 H \perp \mathbf{b}$
Range [K]	50-300	50-300
C [emu.K.(mol Eu) $^{-1}$.Oe $^{-1}$]	8.33	8.31
θ [K]	5.81	5.99
p_{eff} [μ_B]	8.16	8.15

Table 3. Fitting parameters obtained by Curie Weiss analysis from magnetization data of EuGa_2Sb_2 .