Pseudo-Spin Versus Magnetic Dipole Moment Ordering in the Isosceles Triangular Lattice Material \(K_2\text{Er(VO}_4\text{)}_2\)

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(Dated: July 9, 2019)

Spin-1/2 antiferromagnetic triangular lattice models are paradigms of geometrical frustration, revealing very different ground states and quantum effects depending on the nature of anisotropies in the model. Due to strong spin orbit coupling and crystal field effects, rare-earth ions can form pseudo-spin-1/2 magnetic moments with anisotropic single-ion and exchange properties. Thus, rare-earth based triangular lattices enable the exploration of this interplay between frustration and anisotropy. Here we study one such case, the rare-earth double vanadate glasereite material \(K_2\text{Er(VO}_4\text{)}_2\), which is a quasi-2D isosceles triangular antiferromagnet. Our specific heat and neutron powder diffraction data from \(K_2\text{Er(VO}_4\text{)}_2\) reveal a transition to long range magnetic order at \(155 \pm 5\) mK which accounts for all \(Rln2\) entropy. The quasi-2D magnetic order leads to anisotropic Warren-like Bragg peak profiles, and is best described by alternating layers of \(b\)-axis aligned antiferromagnetism and zero moment layers. Our magnetic susceptibility data reveal that \(\text{Er}^{3+}\) takes on a strong \(XY\) single-ion anisotropy in \(K_2\text{Er(VO}_4\text{)}_2\), leading to vanishing moments when pseudo-spins are oriented along \(c\). Thus, the magnetic structure, when considered from the pseudo-spin point of view comprises alternating layers of \(b\)-axis and \(c\)-axis aligned antiferromagnetism.

I. INTRODUCTION

Magnetic frustration has been of interest in condensed matter physics due to the presence of competing interactions which often leads to exotic properties. A two-dimensional (2D) triangular lattice with antiferromagnetically (AFM) interacting Ising spins is the simplest example of geometrical frustration. Wannier found in 1950 that this model has a macroscopically degenerate ground state and the frustration suppresses order down to zero temperature\(^1\). A Quantum Spin Liquid (QSL) state, which exhibits quantum entanglement and fractionalized excitations, was first envisioned by Anderson to exist on a 2D triangular Heisenberg AFM (HAFM)\(^2\). It is now understood that interactions on the 2D triangular HAFM model leads to 120° order\(^3\)\(^-\)\(^5\), but exchange interaction anisotropies or lattice distortions can lead to other interesting phenomena. For example, the isosceles triangular AFM \(\text{Ca}_2\text{CuCl}_4\) was found to be a 1D spin chain and is an example of “dimensional reduction” induced by frustration\(^6\)\(^-\)\(^7\), and anisotropic exchange models on the triangular lattice have been proposed to host QSL phases\(^8\)\(^-\)\(^12\).

Rare-earth based frustrated materials have become of interest due to strong spin orbit coupling and crystal electric field (CEF) effects which can lead to \(S_{g}=\) 1/2 doublets (pseudo-spin-1/2) and anisotropic effective exchange models based on these pseudo-spin-1/2 moments. This makes them ideal to study quantum phases arising from anisotropic exchange. The relationship between the observed magnetic dipole moments (\(\mu_i\)) and the pseudo-spin-1/2 operators \((S_i)\) is given by the \(g\)-tensor: \(\mu_i = g_{ii}S_i\). Depending on the details of the CEF Hamiltonian, the ground state doublet forming the pseudo-spins can have certain \(g\) components become vanishingly small (or in some cases, identically zero due to the symmetry) and thus not appreciable magnetic dipole moment associated with that pseudo-spin direction\(^11\). In the case where the symmetry prevents any dipole moment, these pseudo-spin directions are associated with higher multipoles, such as quadrupoles\(^14\)\(^-\)\(^15\) or octupoles\(^16\)\(^-\)\(^19\).

In terms of the search for quantum magnetic phases based on rare earth ions, \(\text{Yb}^{3+}\) has received the most attention. For instance, \(\text{Yb}_2\text{Ti}_2\text{O}_7\), was proposed as a quantum spin ice material\(^20\)\(^-\)\(^23\) but was later shown to be an unusual ferromagnet with continuum-like scattering\(^24\)\(^-\)\(^26\) that appears to arise from phase competition and non-linear spin wave effects\(^27\)\(^-\)\(^29\). Meanwhile the triangular lattice \(\text{YbMgGaO}_4\) was proposed as a QSL but may instead exhibit a random valence bond state due to Mg/Ga site disorder\(^24\)\(^-\)\(^26\). Frustrated \(\text{Er}^{3+}\) materials are also of interest, and the pyrochlores \((\text{Er}_2\text{B}_2\text{O}_7, B = \text{Ti}, \text{Sn}, \text{Ge}, \text{Pt}, \text{etc.})\)\(^30\)\(^-\)\(^35\), have enjoyed the most attention, but other frustrated geometries realized by \(\text{Er}^{3+}\) are just beginning to be explored\(^36\)\(^-\)\(^41\). Here we study the isosceles triangular material \(K_2\text{Er(VO}_4\text{)}_2\) and show that it has an unconventional magnetic ground state with alternating ordered layers of antiferromagnetic “magnetic dipole active” and “magnetic dipole silent” pseudo-spins.
K$_2$Er(VO$_4$)$_2$ is a member of the rare-earth double vanadate glaserite family, K$_2$RE(VO$_4$)$_2$, where RE = (Sc, Y, Dy, Ho, Er, Yb, Lu, or Tm). Previous studies on rare-earth double phosphate glaserites (K$_2$RE(P$_2$O$_7$)$_2$) have shown that there can exist structural transitions between trigonal and lower symmetry structures of these compounds (i.e. monoclinic) 38,49. While previous reports of K$_2$Er(PO$_4$)$_2$ describe it in terms of a trigonal space group (P$3m1$) at room temperature 50, we have found from powder and single crystal x-ray diffraction and low temperature neutron diffraction that a monoclinic structure (space group C2/c), shown in Fig 1a & b, is appropriate for our samples at all measured temperatures, similar but not identical to K$_2$Er(PO$_4$)$_2$ (which forms in space group P21/m).

II. EXPERIMENTAL METHOD AND RESULTS

The crystal growth of monoclinic K$_2$Er(VO$_4$)$_2$ phase involved two steps. First, powder targeting a stoichiometric product of K$_2$Er(VO$_4$)$_2$ was performed using K$_2$CO$_3$, Er$_2$O$_3$ and (NH$_4$)$_2$VO$_3$. A total of 3 g of components were mixed in a stoichiometric ratio of 3 : 1 : 4 and ground well using an Agate motor and pestle. The powder mixture was then pressed into pellets and heated to 750°C for 80 hours. After the reaction period, the resulted pellets were roughed, ground and checked the purity using powder X-ray diffraction (PXRD). According the PXRD, majority phase was matched with the K$_2$Er(VO$_4$)$_2$ (PDF No. 00-51-0095) with impurities of K$_4$Vo and ErVO$_4$. In the second step, the resulted K$_2$Er(VO$_4$)$_2$ powder was treated hydrothermally to obtain single crystals.

Hydrothermal synthesis was performed using 2.75-inch long silver tubing that had an inner diameter of 0.375 inches. After silver tubes were welded shut on one side, the reactants and the mineralizer were added. Next, the silver ampules were welded shut and placed in a Tuttle-seal autoclave that was filled with water in order to provide appropriate counter pressure. The autoclaves were then heated to 600°C for 14 days, reaching an average pressure of 1.7 kbar, utilizing ceramic band heaters. After the reaction period, the heaters were turned off and the autoclave cooled to room temperature. Crystals were recovered by washing with de-ionized water. In a typical reaction 0.4 g of K$_2$Er(VO$_4$)$_2$ powder was mixed with a mineralizer solution of 0.8 mL of 10 M K$_2$CO$_3$.

Crystals of K$_2$Er(VO$_4$)$_2$ were physically examined and selected under an optical microscope equipped with a polarizing attachment. Room temperature single crystal structures were characterized using a Bruker D8 Venture diffractometer Mo K$_\alpha$ radiation (λ = 0.71073 Å) and a Photon 100 CMOS detector. The Bruker Apex3 software package with SAINT and SADABS routines were used to collect, process, and correct the data for absorption effects. The structures were solved by intrinsic phasing and subsequently refined on F$^2$ using full-matrix least squares techniques by the SHELXTL software package 31. All non-hydrogen atoms were refined anisotropically.

We performed heat capacity measurements from 8 K down to 50 mK (Fig 2) on a 0.41 ± 0.05 mg single crystal (examples shown in Fig 1c) sample using a Quantum Design PPMS with dilution refrigerator insert. We employed two measurement techniques, a typical quasi-adiabatic thermal relaxation measurement with temperature rise \( \Delta T / T \) of 2%, as well as “long pulse” measurements where \( \Delta T / T \) can be as large as 400%, as described in Ref. 52. We find a sharp transition at \( T_N = 155 ± 5 \) mK, much lower than the Curie-Weiss temperature (discussed later), indicating that this system is frustrated as expected, with a frustration parameter of \( f = \theta_{\text{CW}} / T_N \approx 20 \). The total \( C_p(T) \) (not lattice subtracted) reveals a broad peak around 10 K (the shape of which cannot be purely attributed to a power law contribution from acoustic phonon modes), as well as a gradual release of entropy on cooling from 1 K down to \( \sim 150 \) mK, at which temperature a sharp anomaly is observed. The high temperature peak near 10 K is indicative of a low-lying excited CEF multiplet with energy of about 2 meV. The entropy change between 50 mK to 2 K accounts for all the entropy expected from a Kramers CEF ground state doublet (\( R \ln 2 \) per mole Er$^{3+}$, see inset of Fig. 2). Less than 30% of this entropy is released via the sharp anomaly, indicating that short range correlations develop over a broad temperature range above the ordering transition. This is commonly found in low dimensional and frustrated magnets, where ordering is suppressed but is eventually triggered by some subleading energy scale in the Hamiltonian (such as inter-layer interactions in the case of quasi-2D systems) 53. The quasi-2D nature of the magnetism in K$_2$Er(VO$_4$)$_2$ is also confirmed by neutron powder diffraction, as discussed later.

We measured the temperature dependent magnetic susceptibility of K$_2$Er(VO$_4$)$_2$ down to 1.8 K in a 100 Oe field (Fig 3 a) using the MPMS XL Quantum Design SQUID magnetometer on 1.60 ± 0.05 mg and 1.04 ± 0.10 mg of co-aligned single crystals, aligned in the H $\perp$ c and H $\parallel$ c directions respectively. For magnetic fields H $\perp$ c, we find net antiferromagnetic interactions shown by the negative Curie-Weiss temperature $\theta_{\text{CW}}$ $\approx$ $-3$ K obtained by fitting between 2 and 10 K (although this value is highly dependent on the exact fitting range used due to crystal field effects), similar to YbMgGaO$_4$’s $\theta_{\text{CW}}$ $\approx$ $-4$ K. For the magnetic field H $\parallel$ c, the magnetic susceptibility is an order of magnitude less than H $\perp$ c, indicating a strong XY nature of Er$^{3+}$ in this material. Magnetization measurements (Fig 3 b), taken at 1.8 K in a magnetic field up to 5 T, corroborate that K$_2$Er(VO$_4$)$_2$ is a strongly XY system due to the large saturation magnetization for H $\perp$ c. Neither H $\perp$ c or H $\parallel$ c follow a Brillouin function expected for a simple paramagnet, suggesting that there is sig---
significant mixing of the higher CEF states causing the response to be non-paramagnetic. This is particularly obvious for $M_{||c}$ since it starts with a very low moment in zero field. Due to field induced mixing of the excited CEF levels, the saturation magnetization is not a good indicator of the zero-field moment for either direction.

Neutron powder diffraction was performed on the HB-2A beamline at Oak Ridge National Laboratory’s (ORNL) High Flux Isotope Reactor (HFIR). Approximately 2.5 g of crystals were ground into a fine powder, placed into a copper sample can and filled with 10 atm of He gas at room temperature (this technique enables sample thermalization of loose powders below 1 K$^{34}$). Diffraction patterns were obtained from 10 K down to 50 mK. The collimators were set to open-open-12°, and a Ge(113) monochromator provided an incident wavelength of $\lambda = 2.41$ Å. The patterns were collected over a Q-range of $0.18$ Å$^{-1} < Q < 4.64$ Å$^{-1}$ ($4° < 2\theta < 126°$) with count times of 2 hours per scan.

Analysis of the powder diffraction data was performed using the FullProf software suite which implements the Rietveld refinement method$^{55}$. The 10 K data was used to refine the nuclear structure with contributions from the copper cell and aluminum windows masked. Magnetic peaks which could not be indexed within the $K_3\text{Er(VO}_4)_2$ unit cell emerged between 10 K and 400 mK, indicating the presence of magnetic impurities in the sample which we were unable to identify. To remove the signal due to the impurities from the magnetic structure analysis, we subtracted the 400 mK data from the 50 mK data, leaving only the contributions from $K_3\text{Er(VO}_4)_2$ magnetic Bragg peaks (Fig 4). The magnetic peaks indexed gave an ordering wavevector of $\mathbf{k} = (1, 0, 0)$, for which there are two magnetic irreducible representations (IR’s) for a magnetic atom at site (0.5, 0.5, 0.5) found using the SARAhs Representational Analysis software$^{56}$ (Kovalev tables): $\Gamma_1$, with basis vectors $\Psi_{1,2,3}$, and $\Gamma_3$, with basis vectors $\Psi_{1,4,5,6}$. Basis vectors $\Psi_{1,3,5}$ have antiferromagnetic (AFM) spin arrangements in the $ab$ plane which are ferromagnetically (FM) correlated along the $c$-axis (i.e. every layer is identical), with moments pointing along the $a$, $c$, and $b$ axes, respectively. $\Psi_{2,4,6}$ are AFM in the $ab$ plane as well as along the $c$-axis, with moments pointing along the $b$, $a$, and $c$ axes, respectively.

We attempted to fit the magnetic scattering within a single IR, which would be expected for a second order phase transition$^{57}$, however, no linear combination of the basis vectors restricted to a single IR came close to reproducing the observed magnetic structure. A good fit to the data was found with equal contributions from basis vectors $\Psi_2$ (from $\Gamma_1$) and $\Psi_5$ (from $\Gamma_3$), producing alternating layers comprised of AFM order (with moments along $b$), and zero-moment layers (cyan arrows in Fig 5).

It should be noted that all fits lacked perfect agreement with the intensity and shape of the lowest $Q$ magnetic peak, which is indexed as the (100) reflection. The shape of this peak is reminiscent of the Warren line-shape for random 2D layered lattices$^{58}$, having an asymmetric base that extends farther to high $Q$ than it does to low $Q$. In a 2D random layer case, where no correlations exist between layers, the structure factor for $(hkl)$ zone centers is expected to be zero$^{59}$, in contrast to the $(hkl)$ zone centers, which are non-zero and will have this asymmetric shape. For quasi-random 2D layers with some short range correlations between planes, intensity is expected at $(hkl)$ reflections, but peaks will have suppressed intensities and will in principle be broadened compared to a peak arising from long range 3D order. The intensity suppression for $(hkl)$ with $l \neq 0$ appears to be operative in $K_3\text{Er(VO}_4)_2$, but we could not resolve any broadening of these peaks, which implies a correlation length of at least 280 Å. This, combined with the asymmetric peak shape of (100), suggests that quasi-2D magnetic correlations, rather than fully correlated 3D order, builds up below the transition.

III. DISCUSSION

The refined magnetic structure, which lacks ordered moments in every other layer, initially suggests a partially disordered spin state. However, a thermally partially disordered case can be quickly ruled out based on the heat capacity, which produces the full $R \ln 2$ entropy change expected for a fully ordered state upon integrating $C_p/T$ from 50 mK to 1 K. Quantum fluctuations could in principle still produce an average spin of zero on some layers. However, a simpler explanation seems to be possible by considering the inferred $g$-tensor and the presence of antisymmetric exchange, i.e. Dzyaloshinskii-Moriya (DM) interactions, between layers.

DM interactions are not allowed by symmetry between nearest-neighbor sites in the triangular lattice planes (the $ab$ plane), but they are allowed between nearest neighbors along $c$, and Moriya’s rules indicate that the DM vector $\vec{D}$ is constrained to be perpendicular to $\vec{b}$ $^{59}$. This lends itself to the probable pseudo-spin ordering structure illustrated by the black arrows in Fig 5 involving 2D triangular layers alternating between AFM ordered layers with moment along $b$ and $\vec{a}$ $^{62}$. Because of the strong XY single-ion nature of this material ($g_z \sim 0$), the layers with the pseudo-spins pointing along the $c$-axis would carry approximately zero dipole moment and thus appear to be disordered according to probes that are sensitive only to dipole magnetic moments, such as neutron scattering. Similar effects are at play in some rare earth pyrochlores, where the the XY part of the pseudo-spin carries a quadrupolar$^{14,15}$ or octupolar$^{16-19}$ moment but no dipole moment. However, even fully dipolar Kramer’s doubllets can have very small $g$-values in certain directions, such as $\text{Er}_2\text{Sn}_2\text{O}_7$ $^{38}$, $K_3\text{Er(VO}_4)_2$ is one of the clearest examples in which the ordered magnetic structure is a combination of high dipole moment and nearly zero dipole moment pseudo-spin order. Due to the low point symmetry at the $\text{Er}^{3+}$ site (triclinic), the ground state CEF doublet in $K_3\text{Er(VO}_4)_2$ is most likely to be a conventional Kramer’s dou-
AFM interaction of (XY nature of K$_3$ was a linear combination of equal contributions of basis vectors $\Psi_g$ (from $\Gamma_1$) and $\Psi_5$ (from $\Gamma_4$). Magnetic dipole silent layers are proposed to be due to the strong magnetic dipole silent pseudo-spin order along $\textbf{c}$ ordering along the unusual ordered state with AFM magnetic dipole moments $\textbf{g}$ inferred from Curie-Weiss analysis ($\sim 155$ mK). We have performed the first extensive magnetic study of any rare-earth glaserite materials, particularly in their trigonal structural polymorphs, which we speculate is brought about through DM interactions between layers. Inelastic neutron scattering studies of K$_3$Er(VO$_4$)$_2$ could help to validate this model, in particular the strength of this proposed DM interaction, and could also reveal the low lying CEF level. Further studies of other rare earth glaserites, particularly in their trigonal structural polymorphs, would be intriguing, as they could be promising materials for discovering new quantum magnetic phases due to their pseudo-spin-1/2 angular momentum and strong frustration.

**IV. CONCLUSIONS**

We have performed the first extensive magnetic study of any of the rare-earth double vanadate glaserite materials, which form 2D isosceles (or equilateral, in the case of the trigonal polymorphs) triangular lattices. We found an antiferromagnetic transition in K$_3$Er(VO$_4$)$_2$ at 155 mK despite a stronger AFM interaction of 3 K inferred from Curie-Weiss analysis ($f \sim 20$). Susceptibility measurements reveal this material to have strong XY $g$-tensor anisotropy, although coupling to an inferred CEF level at $\sim 2$ meV hinders an estimation of the $g$-tensor via magnetization. The magnetic structure is an unusual ordered state with AFM magnetic dipole moments ordering along the $b$ axis direction in every other layer, and magnetic dipole silent pseudo-spin order along $c$ in the other layers, which we speculate is brought about through a DM interaction between layers. Inelastic neutron scattering studies of K$_3$Er(VO$_4$)$_2$ could help to validate this model, in particular the strength of this proposed DM interaction, and could also reveal the inferred low lying CEF level. Further studies of other rare earth glaserites, particularly in their trigonal structural polymorphs, would be intriguing, as they could be promising materials for discovering new quantum magnetic phases due to their pseudo-spin-1/2 angular momentum and strong frustration.

**Acknowledgments**

We thank Gang Chen for useful discussion. Research conducted at ORNL’s High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy. The work performed in ORNL is partly supported by the DOE, Office of Science, Basic Energy Sciences (BES), Materials Science and Engineering Division. Work performed on synthesis, crystal growth, and x-ray diffraction at Clemson University was funded by DOE BES Grant No. DE-SC0014271.

**Appendix A: Monoclinic Structure Determination**

Crystallographic data for monoclinic K$_3$Er(VO$_4$)$_2$ was determined using single crystal x-ray diffraction, and is shown in Table I. Single crystals of K$_3$Er(VO$_4$)$_2$ were ground into a powder for neutron diffraction using a motor and pestle. A large amount of crystals needed to be ground to achieve a substantial mass for neutron scattering, so the crystals were ground in three batches. These batches were x-rayed separately and then again after the batches were combined. X-ray scattering was performed on a Bruker D8 Discover Davinci diffractometer from $10 < 2\theta < 60$ (Fig 6a.) for approximately 1 second per 0.02 degree.

Using TOPAS Reitveld refinement, the trigonal structure ($P6m1$) was unable to fit all of the peaks, especially the multi-peaked structures that look like $K_{\text{Fe}}$ signals but are not. The monoclinic structure ($C2/c$) found using the single crystal fit parameters fits the majority of peaks quite well, including the multi-peaked structures. Subtle peaks were unable to be fit by either structure refinement indicating a small amount of impurities. These impurities were unable to be identified using EVA’s search/match tool.
FIG. 6: Powder x-ray diffraction for crushed single crystals of K₃Er(VO₄)₂. a) Full scan showing that the monoclinic structure agrees with the majority of the data better than the trigonal structure. b) Close-up of peaks clearly showing that the monoclinic structure fits all peaks, while the trigonal structure fits some peaks well but misses other peaks.

### Appendix B: Further Details on Powder Neutron Diffraction

The nuclear structure was determined from a Rietveld refinement fit to the 10 K data, shown in Fig 7. As with the PXRD data, it is clear that our sample of K₃Er(VO₄)₂ is monoclinic (space group C2/c), as the trigonal structure (space group P3m1) does not fit peaks that the monoclinic structure does. Both structures miss small peaks throughout the fit, indicating the impurities in the sample that were found using PXRD as well.

The low temperature nuclear structure was determined using the 50 mK data while masking the strong magnetic Bragg peaks. We then subtracted out the impurities by subtracting the 400 mK data from the 50 mK data (Fig 8), resulting in only contributions from the K₃Er(VO₄)₂ magnetic structure. The magnetic structure was then able to be fit using a linear combination of basis vectors ψ₁₋₆ from both Γ₁ and Γ₃ IR’s.

A multi-k structure was investigated and found to not match the data. We then attempted to fit the magnetic structure using a single IR, as it was not clear if the transition found in heat capacity was a first- or second-order transition. Example of those fits are shown in Fig 9. When attempting to fit Γ₁ (Γ₃), the fits would not converge unless ψ₁ (ψ₃) was set to zero. Both IR’s lacked agreement with both of the initial peaks, but Γ₁ fit the first peak well which is unexpected due to the 2D nature of this material. Both fits of individual IR’s had peaks which were not seen in the scattering signal, while a combination of

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| Crystallographic data of K₃Er(VO₄)₂ determined by single crystal X-ray diffraction. |
|---------------------------------|
| **Empirical formula** | K₃Er(VO₄)₂ |
| **Formula weight (g/mol)** | 514.44 |
| **Crystal system** | monoclinic |
| **Crystal dimensions, mm** | 0.10 x 0.02 x 0.02 |
| **space group, Z** | C2/c (no. 15), 4 |
| **a, Å** | 10.1956(4) |
| **b, Å** | 5.8650(2) |
| **c, Å** | 15.2050(6) |
| **β,°** | 90.12(1) |
| **Volume, Å³** | 909.21(6) |
| **D(calc), g/cm³** | 3.758 |
| **µ (Mo Kα), mm⁻¹** | 12.543 |
| **F(000)** | 940 |
| **T max, T min** | 0.0000, 0.8169 |
| **2θ range** | 2.679 – 24.990 |
| **reflections collected** | 10581 |
| **data/restraints/parameters** | 781/70/67 |
| **final R(1/1/)(R1, Rw2)** | 0.0372, 0.1144 |
| **final R (all data) K1, R w2** | 0.0374, 0.1144 |
| **GOF** | 1.086 |
| **largest diff. peak/hole, e/Å³** | 1.760/ – 1.155 |

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FIG. 7: Nuclear structure of K₃Er(VO₄)₂ found with neutron scattering. The trigonal structure is unable to fit peaks that the monoclinic structure can. The impurity is also seen in small peaks unable to be fit by either structure, denoted by stars.

FIG. 8: Subtraction of 400 mK scan from 50 mK scan to isolate the magnetic signal from the impurities.

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FIG. 9: Examples of fits to the magnetic structure with individual IR’s.
the IR’s did not. This suggests that the magnetic structure must be a combination of both IR’s and thus a first-order transition.

FIG. 9: Examples of fits using a single irreducible representation. $\Gamma_1$ shows a good fit to the first peak and a poor fit to the second, opposite of what is expected due to the 2D nature of $K_3Er(VO_4)_2$. $\Gamma_3$ has the expected fit to the first two peaks, but both $\Gamma_1$ and $\Gamma_3$ fits give peaks not seen in the data, shown by arrows. Therefore, the best fit comes from a linear combination of $\Gamma_1$ and $\Gamma_3$’s basis vectors, $\psi_2$ and $\psi_5$, respectively.
