Magnetic structures in the rich magnetic phase diagram of 
$\text{Ho}_2\text{RhIn}_8$

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Abstract

The magnetic phase diagram of tetragonal $\text{Ho}_2\text{RhIn}_8$ has similar features to many related systems, revealing a zero field AF1 and a field induced AF2 phases. Details of the magnetic order in the AF2 phase were not yet reported for any of related compounds. In addition, only the $\text{Ho}_2\text{RhIn}_8$ phase diagram contains a small region of the incommensurate zero-field phase AF3. We have performed a number of neutron diffraction experiments on single crystals of $\text{Ho}_2\text{RhIn}_8$ using several diffractometers including experiments in both horizontal and vertical magnetic fields up to 4 T. We present details of the magnetic structures in all the magnetic phases of the rich phase diagram of $\text{Ho}_2\text{RhIn}_8$. The Ho magnetic moments point along the tetragonal $c$-axis in all the phases. The ground-state AF1 phase is characterized by propagation vector $\mathbf{k} = (1/2, 0, 0)$. The more complex ferrimagnetic AF2 phase is described by four propagation vectors $\mathbf{k}_0 = (0, 0, 0)$, $\mathbf{k}_1 = (1/2, 0, 0)$, $\mathbf{k}_2 = (0, 1/2, 1/2)$, $\mathbf{k}_3 = (1/2, 1/2, 1/2)$. The magnetic structure in the small AF3 phase is incommensurate with $\mathbf{k}_{AF3} = (0.5, \delta, 0)$. 

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I. INTRODUCTION

The influence of the dimensionality on the magnetic and superconducting properties of heavy fermion compounds has been studied for a long time. Compounds, with general composition $R_nT_mX_{3n+2m}$ (where $R$ is rare earth, $T$ is a transition metal, $X$ is In or Ga, $n$ and $m$ are integers) are natural candidates for this study because of the possibility of tuning their dimensionality. Heavy fermion superconductivity is observed in some cerium compounds from this series. In general, all of them are made from rare-earth and transition element layers surrounded by cages of indium atoms. Changing the order of these layers along tetragonal $c$ axis leads to the different tetragonal structures with rich ground state properties. In terms of anisotropy, the "218" structure (e.g. Ce$_2$RhIn$_8$) lies in between the well-known 2D "115" structure (e.g. CeCoIn$_5$) and the cubic CeIn$_3$ structure. As the superconductivity is observed only in cerium compounds, studies of the non-cerium analogues helps to focus only on the magnetic structure.

Ho$_2$RhIn$_8$ orders antiferromagnetically below $T_N = 10.9$ K and its magnetic properties are driven mainly by crystal field effects (CEF) together with RKKY interaction. When an external magnetic field is applied along the tetragonal $c$-axis at 2 K, Ho$_2$RhIn$_8$ undergoes two successive magnetic phase transitions. The first one at 2.5 T leads to an intermediate magnetic phase AF2 and the second one at 6 T results in the ferromagnetic order. It is interesting to note, that the magnetization per formula unit in the AF2 phase is just a half of the moment found in the ferromagnetic phase as revealed by magnetization measurements. The magnetic phase diagram of Ho$_2$RhIn$_8$ (see Ref. and Fig. 1) is qualitatively the same as for many other related 115 and 218 compounds with $R = \text{Nd}, \text{Tb}, \text{Dy}$ and Ho which have the $c$-axis as the easy magnetization axis: $R$RhIn$_5$, $R$CoIn$_5$, $R$CoGa$_5$, $R_2$RhIn$_8$, and $R_2$CoGa$_8$. As well as for Ho$_2$RhIn$_8$, the magnetization per formula unit in the field induced AF2 phase in all these compounds is a half of the value in the ferromagnetic phase. The microscopic nature of the magnetic order in AF1 phase was studied in $R$RhIn$_5$ ($R = \text{Nd}, \text{Tb}, \text{Dy}, \text{Ho}$), $R$CoGa$_5$ ($R = \text{Tb}, \text{Ho}$), $R_2$RhIn$_8$ ($R = \text{Nd}, \text{Tb}, \text{Dy}$) and $R_2$CoGa$_8$ ($R = \text{Tb}, \text{Dy}, \text{Ho}$), resulting in the commensurate propagation $k_{115} = (1/2, 0, 1/2)$ in "115" compounds and $k_{218} = (1/2, 1/2, 1/2)$ in "218" compounds. Magnetic structure in AF2 phase was studied only by Hieu in his thesis in NdRhIn$_5$ and DyRhIn$_5$, however no conclusions from this measurements were given and magnetic structure in AF2 phase remains unknown.
FIG. 1. Magnetic phase diagram of Ho$_2$RhIn$_8$. Open points are determined from bulk measurements, filled ones are from current neutron diffraction studies. Lines and shapes are only to guide the eye.

Despite many similarities with Nd, Tb and Dy compounds with related structures, Ho$_2$RhIn$_8$ shows a feature not observed in other related "218" compounds: an additional magnetic phase existing in a narrow temperature region between $T_N = 10.9$ K and $T_1 = 10.4$ K. The phase transition at $T_1$ is clearly visible in specific heat measurements and it was speculated, that is connected with a formation of an incommensurate magnetic phase.

The present paper is focused on the determination of magnetic structures in all three magnetic phases of Ho$_2$RhIn$_8$ using several neutron diffraction experiments. Considering the similar phase diagram and results of magnetization measurements, the magnetic structure in the AF2 phase might be then eventually generalized for the whole class of related 115 and 218 tetragonal compounds.

II. EXPERIMENTAL DETAILS

We used the same Ho$_2$RhIn$_8$ sample as in the previous bulk experiment. The single crystal has the form of a cuboid of approximately 3 x 1 x 0.2 mm size. No deviation from the known crystal structure (space group $P4/mmm$, No. 123) nor any presence of foreign phase were detected by X-Ray diffractometer and EDX microprobe analysis.

Measurements were carried out on the several neutron diffractometers. First, the nuclear structure and the extinction parameters were determined by the D10 instrument at Institute Laue-Langevin (ILL). We used a PG002 monochromator with an incident wavelength $\lambda = 2.36$ Å and a graphite filter before the sample. The orientation matrix and lattice parameters
were refined on the basis of 19 strong nuclear reflections at $T = 2$ K.

Determination of the propagation vectors in the AF1 and AF3 phases was done on Laue diffractometer CYCLOPS\textsuperscript{[12]} at ILL. Measurement of 2 patterns with a different sample rotation at $T = 14$ K and in the ordered state at $T = 1.6$ K took 3 hours per pattern. In addition, a series of 50 patterns was taken in the slow temperature sweep mode (0.1 K/min) in order to determine temperature dependence of the magnetic Bragg peaks and the nature of AF3 phase. Refinement of the Laue data were done in the Esmeralda Laue Suite program\textsuperscript{[14]}

The magnetic phase AF1, as well as the behavior in applied magnetic fields, were measured using the two-axis neutron diffractometer E4 at Helmholtz-Zentrum Berlin, Germany. A focusing monochromator with vertically bent PG crystals was used for the wavelength $\lambda = 2.432$ Å. The scattered intensities were recorded using a 200x200 mm two-dimensional position-sensitive detector (PSD) 896 mm from the sample. The experiment was performed using a He flow cryostat at the temperature range 1.6 - 15 K. First, the sample was loaded into a horizontal-field magnet, HM-2, and aligned with its reciprocal $(h, 0, l)$ plane in the horizontal scattering plane of the instrument. The magnetic field was applied along the easy $c$ axis. In order to extend the number of observable reflections, the sample was realigned and mounted to the vertical-field magnet, VM-2, to have $(h, k, 0)$ plane aligned in the scattering plane of the instrument. The 10 degrees opening angle of the magnet allowed us to reach reflections with index $(h, k, 0.5)$ on the PSD detector.

We used the triple axis spectrometer IN3 at ILL to measure zero-field temperature dependence of magnetic Bragg reflections. The sample was mounted as in E4: with the reciprocal $(h, 0, l)$ plane in the scattering plane and the experiment was performed in the elastic condition at $\lambda = 2.36$ Å.

III. RESULTS AND DISCUSSION

The data from D10 were integrated using the program RACER\textsuperscript{[15]}. Integration of the E4 data was done by a Python script; first cutting out background detector data to a rectangular shape around the observed reflection and then fitting a gaussian profile along the $\omega$-scan. This technique allows us to reduce the background and also to distinguish out-of-plane and in-plane reflections. Data from IN3 were fitted with a Gaussian profile, as this instrument
TABLE I. Refined structural parameters of Ho$_2$RhIn$_8$ at $T=1.6$ K. Space group: $P4/mmm$. $a=4.5648(16)$ Å, $c=11.953(12)$ Å.

| atom  | Wyckoff pos. | x    | y    | z          |
|-------|--------------|------|------|------------|
| Ho    | 2g           | 0    | 0    | 0.3098(3)  |
| Rh    | 1a           | 0    | 0    | 0          |
| In(1) | 2e           | 0    | 0.5  | 0.5        |
| In(2) | 2h           | 0.5  | 0.5  | 0.3086(6)  |
| In(3) | 4i           | 0    | 0.5  | 0.1245(4)  |

has only 1D detector. All intensities were corrected for the Lorentz factor. The obtained raw data were reduced using the program DataRed and the FullProf program was used for the refinement of the structures.

The structural parameters of Ho$_2$RhIn$_8$ were determined on the basis of 68 independent reflections measured on D10; they are summarized in Table I. A single extinction parameter EXT1 (Ext-Model = 1) was used in the FullProf software for correction of extinction. As other neutron measurements were carried out at the similar wavelength on the same piece of crystal, this extinction parameter was used as a fixed value for all E4 and IN3 data refinements.

A. Zero field commensurate structure AF1

All observed diffraction spots on the total Laue pattern obtained in the paramagnetic state can be indexed assuming a tetragonal structure with the space group $P4/mmm$. Their intensity remains unchanged when cooling to the ordered state at $T=1.5$ K, showing no ferromagnetic or $k=(0, 0, 0)$ contribution to magnetic structure in AF1. A large number of purely magnetic reflections appears in the ordered state; all of them can be described by a single propagation vector associated with the X [$k=(1/2, 0, 0)$ and $k'= (0, 1/2, 0)$] point of symmetry. There exist 8 1D irreducible representations associated with this wave vector, but only 6 of them are part of the global reducible magnetic representation of the 2g Wyckoff site occupied by Ho atoms. These can be assigned to 6 possible magnetic structures with the magnetic moments aligned along one of the main crystallographic directions, each
FIG. 2. Crystal structure of the Ho$_2$RhIn$_8$.

with ferro- or antiferromagnetic stacking of the moments on the two Ho positions within the unit cell (positions 1 and 2 in Fig. 2). All possible structures are summarized in Table I.

Magnetic structure refinement using FullProf shows that magnetic moments lie along the $c$ axis, in agreement with magnetization data. The main difference between ++ and +- stacking along the $c$ axis is the existence of the (hk0) magnetic reflections. In case of +- stacking, all these reflections are forbidden. Indeed, we observe a zero magnetic intensity of (hk0) reflections what clearly favors the +- stacking in Ho$_2$RhIn$_8$. Detailed refinement of the intensities of the 7 reflections measured on the E4 diffractometer leads to the size of the magnetic moment $\mu_{AF1} = 6.9(2) \, \mu_B$. Reliability factors of the fit are stated in Table 1 in Ref. [17].

We have observed equally-sized magnetic Bragg reflections associated with both $\mathbf{k} = (1/2, 0, 0)$ and $\mathbf{k}' = (0, 1/2, 0)$ propagation vectors. On the basis of a neutron diffraction experiment it is not possible to distinguish between multi-k structure and the existence of magnetic domains. But the multi-k structure will require moments to lie out of the easy $c$ axis or it will imply existence of the holmium atoms with the zero magnetic moment. Both of these cases are unlikely because of magnetization measurements and therefore we conclude that there exist two magnetic k-domains, corresponding to the propagation vectors $\mathbf{k} =$
TABLE II. Possible magnetic structures in Ho$_2$RhIn$_8$ according to representations theory for given propagation vectors. Moment directions are along the axes stated in the second column, the stacking of the magnetic moments is over 2 unit cells along the $c$ axis on the positions 1 and 2 as shown in Fig. 2.

| prop. vector | moment | direction | $c$ axis | stacking |
|--------------|--------|-----------|---------|---------|
| (0, 0, 0)    | $c$    | $c$       | + + + + |
|              | $a$    | +         |       | - - - - |
|              | $a$    | +         |       | + + + + |
|              | $b$    | +         |       | - - - - |
| (1/2, 0, 0)  | $b$    | +         |       | + + + + |
|              | $c$    | +         |       | - - - - |
|              | $c$    | +         |       | + + + + |
|              | $a$    | +         |       | - - - - |
|              | $a$    | +         |       | + + - - |
| (1/2, 0, 1/2)| $b$    | +         |       | - - - - |
|              | $b$    | +         |       | + + - - |
|              | $c$    | +         |       | - - - - |
|              | $c$    | +         |       | + + - - |
| (1/2, 1/2, 1/2)| $c$ | +         |       | - - - - |
|              | $c$    | +         |       | + + - - |

(1/2, 0, 0) and $\mathbf{k}' = (0, 1/2, 0)$. These domains are equally populated. Resulting magnetic structure is depicted in Fig. 3.

Fig. 4 shows the temperature dependence of the (1/2 0 1) magnetic reflection. Transition temperature $T_1 = 10.4(2)$ K was determined from the inflection point of this dependence. It is in agreement with the value determined from specific heat and is plotted in the phase diagram in Fig. 1.
FIG. 3. Magnetic structure of Ho$_2$RhIn$_8$ in the AF1 phase. Two magnetic domains are shown. Orientation is the same as in Fig. 2.

FIG. 4. Temperature dependence of integrated intensity of (1/2 0 1) reflection in different magnetic fields. Inset shows intensity of the (1/2 0 1) reflection attributed to AF1 phase (circles) together with (1/2 0.036 1) reflection attributed to AF3 phase (squares). Lines are only to guide the eye.

Because all other members of ”218” compounds reveals $k_{218} = (1/2, 1/2, 1/2)$, Ho$_2$RhIn$_8$ is the first member of this series with magnetic domains. Its structure is much more similar to ”115” compounds, having same stacking along the $c$ axis and also the same propagation within $ab$ plane.
B. Field induced structure AF2

In order to determine magnetic structure in the field induced magnetic phase AF2, neutron diffraction experiments were carried out in horizontal and vertical magnet in a field of 4 T. A thorough search in the reciprocal space leads to observation of magnetic reflections described by six propagation vectors: $k_0 = (0, 0, 0)$, $k_1 = (1/2, 0, 0)$, $k'_1 = (0, 1/2, 0)$, $k_2 = (1/2, 0, 1/2)$, $k'_2 = (0, 1/2, 1/2)$ and $k_3 = (1/2, 1/2, 1/2)$, where $k_{1,2}$ and $k'_{1,2}$ correspond to the different magnetic domains. Reciprocal space positions $(1/2, 1/2, l)$ and $(h, k, 1/2)$ were measured for a longer time and no magnetic reflections were found there. The magnetic unit cell size is thus $2a$, $2b$, $2c$. The sum of the magnetic moments associated with $k_1$, $k_2$ and $k_3$ within the magnetic unit cell is always zero, as they are always propagating within the $ab$ plane canceling out moments at the $2g$ Wyckoff site. The magnetization measurement clearly shows that the overall magnetic moment in the AF2 phase amounts to the half of the magnetic moment of Ho in ferromagnetic state above 6 T ($\approx 4 \mu_B$)\(^3\). This moment does not propagate and is associated with the ferromagnetic component ($k_0$) of the AF2 phase. Refinement of the measured ferromagnetic intensities using the FullProf software confirmed this prediction and leads to the magnetic moment $\mu_{k_0} = 3.6(4) \mu_B$ in agreement with magnetization measurements.

We have done symmetry analysis based on representations theory for the remaining propagation wave vectors, as in case of AF1. Possible directions of the magnetic moments are summarized in Table II. For structures with $k_1$ and $k_2$ there exists always 6 allowed 1D irreducible representations. In case of $k_3$, there is a general possibility for the moment to lie in any direction within $ab$ plane (detailed symmetry and magnetic group analysis for this structure and propagation is discussed in Ref. [10]). Taking into account the fact, that all moments in AF1 point along $c$ axis and a clear field induced spin flip behavior is observed, we can consider that magnetic moments associated with all the wave vectors $k$ in AF2 point also along $c$ axis.

In order to construct possible magnetic structures, we will now focus on the magnetic spin arrangement within (002\(_{Ho}\)) plane (highlighted in red in Fig. 2). This consideration simplifies the problem to 2 dimensions. There are four magnetic positions within this plane in magnetic unit cell (marked A-D in Fig. 2), all corresponding to one atom site in nuclear unit cell. There can exist 4 propagation vectors in maximum: $k_{0,\text{plane}} = (0, 0)$, $k_{1,\text{plane}} =$
TABLE III. Possible magnetic structures in AF2 phase based on propagation vectors analysis. Stacking along $c$ axis has same meaning as in Table II.

| $c$ axis stacking on site A (see Fig. 2) | model 1 | model 2 |
|----------------------------------------|---------|---------|
| $k_0 = (0, 0, 0)$                      | $+++$   | $+++$   |
| $k_1 = (1/2, 0, 0)$                    | $+++$   | $+-+-+$ |
| $k_2 = (0, 1/2, 1/2)$                  | $--++$  | $+-+-+$ |
| $k_3 = (1/2, 1/2, 1/2)$                | $++--$  | $++--$  |
| Overall stacking                       | $+++$   | $++--$  |

$(1/2, 0)$, $k_{2,plane} = (0, 1/2)$ and $k_{3,plane} = (1/2, 1/2)$. Considering only spin flip scenario, the total magnetic moments on all 4 sites $\mu_{A-D}$ must have the same amplitude. If we neglect the change of the magnitude of the magnetic moment and assume that the magnetic moments are along $c$ axis, there exist the only possible solution:

$$\mu_{k_0} = \mu_{k_1} = -\mu_{k_2} = \mu_{k_3},$$

(1)

$$\mu_A = -\mu_B = \mu_C = \mu_D = 2\mu_{k_0},$$

(2)

which means that the component associated with $k_2$ has an opposite sign with respect to all other components and one of the 4 magnetic moments within the plane is flipped. For details of the derivation, see Ref. [17].

Extending from 2D case to real Ho$_2$RhIn$_8$ structure brings much more options (six propagation vectors, each with two possible stackings along $c$ axis). Taking into account fact, that total magnetic moment at one site cannot be bigger than full magnetic moment of Ho (10 $\mu_B$) and $\mu_{k_0} = 3.6(4)\mu_B$, only two independent models summarized in Table III and depicted in Fig. 5 are possible. They are distinguishable on the same principle as for AF1 phase - on the basis of the existence of the reflections (hk0) for propagation vector $k_1$. These reflections are forbidden in the model 2. As we indeed did not observe any of these reflections, the correct model describing the magnetic structure of Ho$_2$RhIn$_8$ in the AF2 phase is the model 2. As well as in AF1, there will exist two magnetic k-domains. The resulting magnetic structure is shown in Fig. 6.

Quantitative refinement using the FullProf software confirmed described results and leads...
FIG. 5. Possible magnetic structures in AF2 phase with highlighted ferromagnetically ordered planes. Model 1 consists of ferromagnetic and antiferromagnetic (00l) planes. Model 2 is more complicated revealing ferromagnetically ordered atoms in some kind of zig-zag planes. Orientation is the same as in Fig. 2.

To the magnetic moments associated with different propagation vectors as follows: $\mu_{k_0} = 3.6(4) \mu_B$, $\mu_{k_1} = 3.7(3) \mu_B$ and $\mu_{k_2} = -4.0(2) \mu_B$. The amplitude of the magnetic moments described by the propagation vector $k_3$ was not possible to determine, since due to the construction of magnets, we have reached only one magnetic reflection associated with this propagation. Reliability factors of the fitting procedure are stated in Table 1 in Ref. 17. All three determined amplitudes satisfy equation (1) within their errors. The overall amplitude of magnetic moments is $\mu_{AF2} = 7.5(5) \mu_B$, which is calculated from equation (2) taking $\mu_{k_0}$ as the mean of all three refined amplitudes of magnetic moments. The value of $\mu_{AF2}$ is slightly bigger than $\mu_{AF1}$. This increase is due to impact of the 4 T external magnetic field and is in agreement with the measured magnetization curves.

To clarify the location of the phase boundaries and verify consistency of the data from vertical and horizontal magnet, several reflections were followed with the changing magnetic
field (Fig. 7). The transition from AF1 to AF2 phase is illustrated by a strong decrease of intensity of the 1/2 0 1 and 1/2 0 2 reflections together with increase of the intensity at the positions of the nuclear peaks and peaks described by the propagation vectors $k_2$ and $k_3$. Temperature dependence of (1/2 0 1) reflection in the fields of 2 and 3 T is depicted in Fig. 4. The shape of the curve in 0 T and 2 T corresponds to each other showing the same ordering mechanism as both are entering the AF1 phase. The appearance of the AF1 phase within a limited temperature range in the field of 3 T, indicated by bulk measurements (Fig. 1), was not observed. This can be explained by absence of long-range order in the narrow AF1 phase region just below the ordering temperature in 3 T. Points from the measured temperature and the field dependencies are included in the phase diagram in Fig. 1.

As this is the first solved AF2 structure in the family of $R_2TIn8$ and $RTIn_5$ compounds, we cannot compare results to the related compounds. We suppose that, due to the similar phase diagrams, related compounds from “218” family will perform the same flipping mechanism during metamagnetic transition from AF1 to AF2, consisting of the flip of 1/4

![Diagram of magnetic structure](image)

**FIG. 6.** The magnetic structure of Ho$_2$RhIn$_8$ in the AF2 phase. Two magnetic domains are equally populated. The orientation is the same as in Fig. 2.
of the magnetic moments. The same could be applied with small modification to ”115” compounds, as the AF1 structure in Ho₂RhIn₈ is very similar to the known ”115” magnetic structures. On the basis of the magnetization measurements, Hieu suggested several possible magnetic structures in AF2 phase for ”115” compounds. One of these magnetic structures (Fig. 5.69(c) in Ref. 8) corresponds to the model determined for the AF2 phase in Ho₂RhIn₈.

C. Incommensurate structure AF3

Magnetic intensity in the AF3 phase is illustrated in Fig. 8 which shows the same small portion of Laue diagrams taken at different temperatures. At 11.1 K, above the Néel temperature, there is no significant intensity. At 10.6 K two satellites at incommensurate position appear together with very weak trace of a commensurate (1/2 0 1) reflection. The intensity of the commensurate reflection starts to grow and at 10.1 K there are clearly both commensurate and incommensurate reflections visible. At 9.6 K is AF3 phase completely vanished.
FIG. 8. Detail of the region around 0.5 0 1 reflection in the Laue pattern taken at different temperatures.

Integrated cut along the curves going through all three reflections are shown in Fig. 9. The same behavior was observed also around other strong magnetic reflections and the magnetic peaks on the incommensurate positions were indexed with the propagation vector $k_{AF3} = (1/2, \delta, 0)$, where $\delta = 0.036(3)$. However, as the Laue patterns were taken during temperature sweep and all spots are well localized in reciprocal space at constant positions, $\delta$ is temperature independent. This can be also seen on Fig. 9. Determined data are consistent with $T_N = 10.9$ K determined from specific heat measurements.\[3

Formation of the incommensurate zero-field phase is unique within "218" and "115" compounds, but can be found in the tetragonal compounds structurally related to the other well known heavy fermion superconductor CeCu$_2$Si$_2$ (e.g. UCu$_2$Si$_2$\[15\]). A very small value of the incommensurate component of the propagation vector implicate modulation period involving about 27 holmium atoms. Such a long modulation can be explained by formation of a spin density wave phase.
IV. CONCLUSION

We have determined the magnetic structures in Ho$_2$RhIn$_8$ by means of neutron diffraction experiments. In the zero-field ordered state, the magnetic order is characterized by a single propagation vector $\mathbf{k}_{AF1} = (1/2, 0, 0)$ with antiferromagnetic coupling of Ho moments along $c$ axis and the amplitude of the magnetic moment 6.9(2) $\mu_B$. Before entering this ground-state commensurate phase, there exists a small temperature region where incommensurate phase with propagation $\mathbf{k}_{AF3} = (1/2, 0.036, 0)$ develops. In the applied magnetic field along $c$ axis magnetic structure transforms by spin-flipping of the 1/4 of magnetic moments to another commensurate phase with the amplitude of magnetic moment 7.5(5) $\mu_B$ (in $B = 4$ T). Similar flipping behavior is expected also in the other related compounds with the same phase diagram.

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See Supplemental Material at [URL will be inserted by publisher] for detailed derivation of the in-plane solution of a magnetic moment arrangement in $2a \times 2b$ magnetic unit cell and reliability factors of the FullProf fitting routine.

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