Magnetic order in the chemically-substituted frustrated antiferromagnet CsCrF$_4$

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The effect of chemical substitution on the ground state of the geometrically frustrated antiferromagnet CsCrF$_4$ has been investigated through a neutron powder diffraction experiment. Magnetic Fe-substituted CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and nonmagnetic Al-substituted CsCr$_{0.98}$Al$_{0.02}$F$_4$ samples are measured, and magnetic Bragg peaks are clearly observed in both samples. Magnetic structure analysis revealed a 120° structure having a magnetic propagation vector $k_{\text{mag}} = (0, 0, 1/2)$ in CsCr$_{0.94}$Fe$_{0.06}$F$_4$. For CsCr$_{0.98}$Al$_{0.02}$F$_4$, a quasi-120° structure having $k_{\text{mag}} = (1/2, 0, 1/2)$ is formed. It is notable that the identified magnetic structure in CsCr$_{0.94}$Fe$_{0.06}$F$_4$ belongs to a different phase of ground states from those in CsCr$_{0.98}$Al$_{0.02}$F$_4$ and the parent CsCrF$_4$. These results suggest that the Fe substitution strongly influences the ground state of CsCrF$_4$.

I. INTRODUCTION

Geometrically frustrated magnets have attracted great interest in condensed matter physics because of their exotic magnetic states induced by macroscopic degeneracy of magnetic states at low temperatures [1,2]. Since the macroscopic degeneracy in the low-energy region can be lifted even by small perturbations, geometrical frustration highlights small effects such as single-ion anisotropy [3,4], the Dzyaloshinskii-Moriya interaction [5,6], magnetic dipole-dipole interaction [7,8], exchange randomness [9–12], and site dilution [13–15]. These may play key roles in determining ground states in frustrated magnets.

The equilateral triangular spin tube antiferromagnet CsCrF$_4$ is one of the intriguing species in geometrically frustrated magnets [16,17]. It crystallizes in a hexagonal structure with the space group $P6_2m$ as illustrated in Fig. 1. The magnetic properties are due to $S = 3/2$ Cr$^{3+}$ ions. The unique feature of equilateral triangles formed by CrF$_6$ octahedra are stacked along the crystallographic $c$ axis, forming triangular spin tubes. These tubes magnetically couple with one another and form the kagome-triangular lattice in the $ab$ plane [18,19]. Magnetic susceptibility measurements revealed the Curie-Weiss temperature $\theta_{\text{CW}} = -145$ K and a broad maximum at $T \sim 60$ K indicative of developing short-range antiferromagnetic spin correlations [16,17]. Due to the geometrical frustration and low dimensionality of the triangular spin tube, no clear evidence of a magnetic phase transition was found in thermodynamic and magnetic measurements [16,17,20,22].

In a breakthrough, recent neutron powder diffraction study identified long-range magnetic order of CsCrF$_4$ below 2.8 K. The magnetic moments form a quasi-120° structure in the $ab$ plane [23]. The 120° structure propagates antiferromagnetically along the $a$ and $c$ axes with a magnetic propagation vector $k_{\text{mag}} = (1/2, 0, 1/2)$. Discussion of ground states in the kagome-triangular lattice model suggested that the identified 120° structure originates from a ferromagnetic intertube coupling, the Dzyaloshinskii-Moriya interaction, and a strong in-plane single-ion anisotropy. In addition, it was found that the ground state of CsCrF$_4$ is close to the boundary on the magnetic phase diagram in the kagome-triangular lattice model [23]. This suggests that small perturbations may induce various types of magnetic states in CsCrF$_4$.

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Chemical substitution controls the magnetic state in CsCrF$_4$ [24, 25]. Thermodynamic and magnetic measurements for chemically substituted CsCr$_{1-x}$Fe$_x$F$_4$ and CsCr$_{1-x}$Al$_x$F$_4$ showed that the magnetic state is significantly influenced by the chemical composition [25]. An antiferromagnetic transition was clearly observed at 4.5 K for $x = 0.06$ in the magnetic Fe-substituted compound, and the substituted superexchange bond Cr$^{3+}$-$F^-$.Fe$^{3+}$ enhanced the in-plane magnetic anisotropy. A glasslike transition appeared at about 5 K for the nonmagnetic Al-substituted compound. In the present paper, we investigate long-range magnetic ordering in chemically substituted frustrated antiferromagnet CsCrF$_4$. Magnetic structures of CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and CsCr$_{0.98}$Al$_{0.02}$F$_4$ are identified by a combination of neutron powder diffraction experiments and magnetic structure analysis. The most notable result is that the Fe-substitution effectively turns the ferromagnetic intertube coupling antiferromagnetic.

II. EXPERIMENTAL DETAILS

Polycrystalline samples of CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and CsCr$_{0.98}$Al$_{0.02}$F$_4$ were prepared by a solid-state reaction method [16, 23]. The powder samples were loaded in vanadium-made containers, which were in turn installed in a conventional liquid $^4$He cryostat. Neutron diffraction measurements were performed at the high resolution powder diffractometer ECHIDNA [26, 27] installed at the OPAL research reactor operated by the Australian Nuclear Science and Technology Organisation (ANSTO). We chose a Ge(331) monochromator to obtain neutrons with a wavelength of 2.4395 Å, and used the open-open-5' configuration. Temperatures were set at 10 K and 1.5 K. The neutron diffraction data were analyzed by the Rietveld method with the FULLPROF software [28]. Candidates for magnetic structures compatible with the lattice symmetry were obtained by the SARA$^h$ software [29]. We used the VESTA software [30] for drawing the crystal structures and magnetic structures.

III. RESULTS AND ANALYSIS

Figures 2(a) and 2(b) show neutron powder diffraction profiles at 10 K for CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and CsCr$_{0.98}$Al$_{0.02}$F$_4$, respectively. These are reasonably fitted by the hexagonal structure with the space group $P6_2m$. Obtained profile factors are $R_{wp} = 7.33\%$ and $R_w = 3.70\%$ for CsCr$_{0.94}$Fe$_{0.06}$F$_4$, and $R_{wp} = 9.26\%$ and $R_w = 5.01\%$ for CsCr$_{0.98}$Al$_{0.02}$F$_4$. The refined lattice and structural parameters (Table I) are consistent with the previous results measured by x-ray powder diffraction experiments [24, 25]. We conclude that the crystal structures are retained at low temperatures.

Figure 3 shows neutron diffraction profiles at 1.5 and 10 K, which are below and above the transition temper-

![Neutron powder diffraction profiles for (a) CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and (b) CsCr$_{0.98}$Al$_{0.02}$F$_4$ measured at 10 K. Red squares and black curves show the experimental data and simulations, respectively. Vertical bars indicate the position of the nuclear Bragg peaks. Solid curves below the bars show the difference between the data and simulations.]

**TABLE I.** Results of the structural refinement in space group $P6_2m$ of the neutron powder diffraction profiles measured at $T = 10$ K for CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and CsCr$_{0.98}$Al$_{0.02}$F$_4$.

|                  | CsCr$_{0.94}$Fe$_{0.06}$F$_4$ |                  | CsCr$_{0.98}$Al$_{0.02}$F$_4$ |
|------------------|-------------------------------|------------------|-------------------------------|
|                  | $a$ (Å) 9.56402(7)            |                  |                  |
|                  | $c$ (Å) 3.85832(3)            |                  |                  |
| Cs (3g)          | (0.57202(12), 0, 1/2)         |                  |                  |
| Cr and Fe (3f)   | (0.22456(23), 0, 0)           |                  |                  |
| F (3f)           | (0.83226(14), 0, 0)           |                  |                  |
| F (3g)           | (0.22024(15), 0, 1/2)         |                  |                  |
| F (6j)           | (0.43914(10), 0.16142(11), 0)|                  |                  |
nature observed in the magnetic susceptibility data. In both samples, diffuse scattering is observed at 10 K in the range of $20° \leq 2\theta \leq 40°$, and it is suppressed below the transition temperature. This behavior is the same as in CsCrF$_4$, and indicates that the short-range spin correlations develop at 10 K. For CsCr$_{0.94}$Fe$_{0.06}$F$_4$, we clearly see additional peaks at 1.5 K, indicating the long-range magnetic order. Additional peaks are also visible in CsCr$_{0.98}$Al$_{0.02}$F$_4$ even though their intensities are weak. This result suggests that the anomaly observed at 5 K in the magnetic susceptibility measurements corresponds to weak long-range magnetic ordering rather than the glasslike transition. Remarkably, the peaks for CsCr$_{0.94}$Fe$_{0.06}$F$_4$ are observed at different scattering angles from those in CsCrF$_4$, while the peak positions in CsCr$_{0.98}$Al$_{0.02}$F$_4$ are the same with CsCrF$_4$. Indexing the observed magnetic Bragg peaks results in the magnetic propagation vectors $k_{\text{mag}} = (0, 0, 1/2)$ for CsCr$_{0.94}$Fe$_{0.06}$F$_4$ and $k_{\text{mag}} = (1/2, 0, 1/2)$ for CsCr$_{0.98}$Al$_{0.02}$F$_4$.

To determine magnetic structures that are compatible with the space group symmetry, we performed representation analysis. We assume that a magnetic structure is described by a single irreducible-representation (IR). For CsCr$_{0.94}$Fe$_{0.06}$F$_4$, the representation analysis with the space group $P62m$ and the propagation vector $k_{\text{mag}} = (0, 0, 1/2)$ leads to five IRs. The details of the IRs and corresponding basis vectors are listed in Table I. From the Rietveld refinement, a magnetic structure described by $\Gamma_2$ gives excellent agreement with the experimental data, as shown in Fig. 1(a). $R$ factors for the whole profile are $R_{\text{wp}} = 8.67\%$ and $R_e = 3.86\%$. The magnetic $R$ factor is $R_{\text{mag}} = 7.40\%$. Note that small peaks at $2\theta = 22°$ and $58°$ are likely due to nonmagnetic impurities because they are also observed at 10 K. In the identified magnetic structure, the magnetic moments form a $120°$ structure in the $ab$ plane, and they propagate antiferromagnetically along the $c$ axis, as displayed in Figs. 1(b) and 1(c). The averaged magnitude of the magnetic moment is evaluated to be $1.66(1) \mu_B$. Since an effective magnetic moment for Cr$_{0.94}$Fe$_{0.06}$ is provided by $3.12 \mu_B (= 0.94 \times 3 \mu_B + 0.06 \times 5 \mu_B)$, the refined moment size is much smaller than the effective one. This is the same result as that in the parent CsCrF$_4$. This implies that the magnetic moment strongly fluctuates even at 1.5 K due to the geometrical frustration and low dimensionality.

For CsCr$_{0.98}$Al$_{0.02}$F$_4$, the representation analysis with the space group $P62m$ and the propagation vector $k_{\text{mag}} = (1/2, 0, 1/2)$ leads to splitting of the three equi-
FIG. 5. Refined diffraction profiles for CsCr$_{0.98}$Al$_{0.02}$F$_4$ at 1.5 K. The IRs of the magnetic structure for the simulations are (a) $\Gamma_2$ and (b) $\Gamma_4$, respectively. Red squares and black curves show the experimental data and simulations, respectively. Vertical bars and triangles indicate the position of the nuclear and magnetic Bragg peaks. Solid curves below the triangles show the difference between the data and simulations. The magnetic structures of CsCr$_{0.98}$Al$_{0.02}$F$_4$ with (c) $\Gamma_2$ and (d) $\Gamma_4$.

FIG. 6. (a) Superexchange interactions between the Cr$^{3+}$ ions in 180° and 90° bonds via the F$^-$ ion. (b) Superexchange interactions between the Cr$^{3+}$ and Fe$^{3+}$ ions in 180° and 90° bonds via the F$^-$ ion. [(c) and (d)] Spin structures with an antiferromagnetic interaction on an equilateral triangle.

IV. DISCUSSION

In the magnetic structure analysis, the 120° structure having $R_{\text{mag}} = (0, 0, 1/2)$ is found for CsCr$_{0.94}$F$_{0.06}$F$_4$. In the identified structure, the intertube spin configuration is different from that in the parent CsCrF$_4$, but the intratube structure is the same. Let us discuss Fe-substitution effect on exchange interactions. According to the Goodenough-Kanamori rules [31][32], superexchange interactions between the Cr$^{3+}$ ions via the F$^-$ ion are antiferromagnetic for a 180° bond and ferromagnetic...
for a 90° bond as displayed in Fig. 6(a). Once the Cr\textsuperscript{3+} ion is substituted by the Fe\textsuperscript{3+} ion, the superexchange interactions in the 180° and 90° bonds are turned into ferromagnetic and antiferromagnetic ones, respectively [Fig. 6(b)]. Since the bond angles of the nearest-neighbor exchange paths along the c axis, \( J_0 \), and in the ab plane, \( J_1 \), (see Fig. 1) are 178° and 148° in CsCrF\textsubscript{4}, their exchange interactions likely turn antiferromagnetic into ferromagnetic by the Fe-substitution. However, the identified magnetic structure in the triangular tube retains the same structure as that in CsCrF\textsubscript{4}. This means that the bond substitution in the intratube coupling has no real effect other than to create a small number of ferromagnetically coupled pairs.

On the contrary, the spin configuration between the spin tubes is totally different from that in CsCrF\textsubscript{4}. In CsCr\textsubscript{0.94}Fe\textsubscript{0.06}F\textsubscript{4}, the magnetic propagation vector in the kagome-triangular plane \( k_\text{2D} \) is (0, 0). It contrasts with \( k_\text{2D} = (1/2, 0) \) in CsCrF\textsubscript{4}. This indicates that the substitution drastically changes the ground state even though intertube exchange paths are complicated. In fact, according to the phase diagram of magnetic structures for the kagome-triangular lattice model \([10, 23]\), 120° structures having \( k_\text{2D} = (0, 0) \) and \( (1/2, 0) \) require antiferromagnetic and ferromagnetic intertube couplings, respectively. We note that in the phase diagram the variation of the in-plane anisotropy is more sensitive to magnetic structure analysis reveals that the Fe-substituted sample exhibits a 120° structure having \( k_\text{mag} = (0, 0, 1/2) \), and the Al-substituted one has a quasi-120° structure having \( k_\text{mag} = (1/2, 0, 1/2) \). Importantly, the magnetic structure in CsCr\textsubscript{0.94}Fe\textsubscript{0.06}F\textsubscript{4} differs from that in the parent CsCrF\textsubscript{4}. This result suggests that the ground state in CsCrF\textsubscript{4} is more sensitive to magnetic rather than nonmagnetic substitution on the Cr site. Further studies of magnetic excitation for the Fe-substituted CsCrF\textsubscript{4} would be important to elucidate the spin interactions.

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**TABLE II. Basis vectors for the space group \( P\overline{6}2m \) with \( k_\text{mag} = (0, 0, 1/2) \). The atoms are defined according to Cr1: (0.2246, 0, 0), Cr2: (0, 0.2246, 0), Cr3: (0.7754, 0.7754, 0).**

| IRs | Basis Vectors \([m_a, m_b, m_c]\) |
|-----|----------------------------------|
| \( \Gamma_2 \) | \( \Psi_1 \) \( [1 \ 0 \ 0] \) \( [0 \ 1 \ 0] \) \( [-1 \ -1 \ 0] \) |
| \( \Gamma_4 \) | \( \Psi_2 \) \( [0 \ 0 \ 1] \) \( [0 \ 0 \ 1] \) \( [0 \ 0 \ 1] \) |
| \( \Gamma_4 \) | \( \Psi_3 \) \( [1 \ 2 \ 0] \) \( [-2 \ -1 \ 0] \) \( [1 \ -1 \ 0] \) |
| \( \Gamma_5 \) | \( \Psi_4 \) \( [0 \ 0 \ 2] \) \( [0 \ 0 \ -1] \) \( [0 \ 0 \ -1] \) |
| \( \Gamma_5 \) | \( \Psi_5 \) \( [0 \ 0 \ 0] \) \( [0 \ 0 \ -\sqrt{3}] \) \( [0 \ 0 \ \sqrt{3}] \) |
| \( \Gamma_6 \) | \( \Psi_6 \) \( [2 \ 0 \ 0] \) \( [0 \ -1 \ 0] \) \( [1 \ 1 \ 0] \) |
| \( \Psi_7 \) | \( [0 \ 1 \ 0] \) \( [1/2 \ 1/2 \ 0] \) \( [-1/2 \ 0 \ 0] \) \( +i[\sqrt{3}/2 \ \sqrt{3}/2 \ 0] \) \( +i[\sqrt{3}/2 \ 0 \ 0] \) |
| \( \Psi_8 \) | \( [0 \ 0 \ 0] \) \( [0 \ -\sqrt{3}] \) \( [-\sqrt{3} \ -\sqrt{3}] \) |
| \( \Psi_9 \) | \( [1/2 \ 1/2 \ 0] \) \( [-1/2 \ 0 \ 0] \) \( [0 \ 1 \ 0] \) \( +i[\sqrt{3}/2 \ -\sqrt{3}/2 \ 0] \) \( +i[-\sqrt{3}/2 \ 0 \ 0] \) |

**V. CONCLUSION**

In conclusion, we have studied magnetic orders in magnetic Fe- and nonmagnetic Al-substituted CsCrF\textsubscript{4} through a neutron powder diffraction experiment. Magnetic structure analysis reveals that the Fe-substituted sample exhibits a 120° structure having \( k_\text{mag} = (0, 0, 1/2) \), and the Al-substituted one has a quasi-120° structure having \( k_\text{mag} = (1/2, 0, 1/2) \). Importantly, the magnetic structure in CsCr\textsubscript{0.94}Fe\textsubscript{0.06}F\textsubscript{4} differs from that in the parent CsCrF\textsubscript{4}. This result suggests that the ground state in CsCrF\textsubscript{4} is more sensitive to magnetic rather than nonmagnetic substitution on the Cr site. Further studies of magnetic excitation for the Fe-substituted CsCrF\textsubscript{4} would be important to elucidate the spin interactions.

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TABLE III. Basis vectors for the space group $P\bar{6}2m$ with $k_{\text{mag}} = (1/2, 0, 1/2)$. The atoms are defined according to Cr1: $(0.2233, 0, 0)$, Cr2: $(0, 0.2233, 0)$, Cr3: $(0.7767, 0.7767, 0)$.

| IRs Basis Vectors $[m_a m_b m_c]$ | Cr1 | Cr2 |
|----------------------------------|-----|-----|
| $\Gamma_1 \Psi_1^{(1)}$ | $[0 
0 1]$ | $[0 
0 1]$ |
| $\Gamma_2 \Psi_2^{(1)}$ | $[1 
0 0]$ | $[1 
1 0]$ |
| $\Psi_1^{(1)}$ | $[0 
1 0]$ | $[0 
1 0]$ |
| $\Gamma_3 \Psi_3^{(1)}$ | $[0 
0 1]$ | $[0 
0 -1]$ |
| $\Gamma_4 \Psi_4^{(1)}$ | $[0 
1 0]$ | $[-1 
-1 0]$ |
| $\Psi_1^{(2)}$ | $[0 
1 0]$ | $[0 
1 0]$ |
| $\Gamma_2 \Psi_2^{(2)}$ | $[0 
-1 0]$ | |
| $\Gamma_3 \Psi_2^{(2)}$ | $[0 
0 2]$ | |
| $\Gamma_4 \Psi_3^{(2)}$ | $[2 
1 0]$ | |

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