POLARIZATION, SPIN CHIRALITY AND CANTING, TOROIDAL MOMENT INDUCED BY DZIALOSHINSKY-MORIYA INTERACTION IN $V_3$ NANOMAGNET IN TRANSVERSE MAGNETIC FIELD

Moisey I. Belinsky

School of Chemistry, Tel-Aviv University, Tel Aviv, Ramat Aviv 69978, Israel, belinski@post.tau.ac.il

Abstract

Spin canting, electric polarization, spin chirality, toroidal and magnetic moments are investigated in the spin-frustrated $V_3$ single-molecular magnet ($V_3$) with the out-of-plane ($D_x$) and in-plane ($D_x, D_y$) Dzialoshinsky-Moriya (DM) interaction in transverse magnetic field $B_z \perp Z$ lying in the triangle XY plane perpendicular to the trigonal Z axis. The spin current (or inverse DM) mechanism of polarization $P$ is the driving force of the polarization $P_z(B_z)$ induced by the $D_x$ coupling in the field $B_z$. The inverse DM mechanism leads to polarization $P_z(B_z)$ which increases nonlinearly with increasing field $B_z$, reaches a maximum at the avoided level crossing field $B_{ac}$ and then gradually decreases in high fields. In transverse field $B_z$, the $D_x$ coupling in $V_3$, results also in the field-induced in-plane toroidal moment $T_y(B_z)\parallel Y$. The origin of $P_z(B_z)$ and $T_y(B_z)$ is the large out-of-plane spin fluctuations induced by the $D_x$ coupling. The correlations between the polarization, toroidal and magnetic moments, spin chirality and spin canting in transverse field were investigated in detail. The dynamics of the individual $S_1, S_2, S_3$ spins in the ground and excited states of the avoided level crossing structure in transverse field $B_z (B_x, B_y)$ significantly differs from the spin dynamics in the field $B_z \parallel Z$. The field-induced spin canting in $B_z$ includes large canting of the ($S_1, S_2$) and $S_3$ spins in opposite directions which is accompanied by the significant different change of the $M_i$ projections. The coupling between the vector chirality $\kappa$ and transverse field $B_z$ is non-linear. The vector chirality $\kappa_z(B_z)$ describes the in-plane fluctuations and rotations of the $S_1, S_2$ spins in transverse field $B_z$. The $D_y$ coupling in the $V_{3y}$ system results in the field-dependent toroidal magnetic moment $T_y(B_z)\parallel X$ in $B_z$. Under the field $B$ rotation in the XZ plane, the polarization $P_z(B)$ demonstrates the reduction of the magnitude, while the toroidal moment $T$ exhibits the $T_y(B_z)\rightarrow T_z(B_z)$ flop and reduction. The DM $V_3$ nanomagnets are the cluster analogs of multiferroics.

1. Introduction

Clusters and rings of transition metal ions have attracted a great interest as nanoscale molecular magnets and the elements for potential application in molecule-based quantum computation and magnetolectronics [1-10]. The Dzialoshinsky-Moriya [11, 12]
(DM) interaction $\mathbf{H}_{\text{DM}} = \sum \mathbf{D}_{ij} [\mathbf{S}_i \times \mathbf{S}_j]$ results in the zero-field splitting (ZFS) of the spin-frustrated $2(S=1/2)$ states [13-33, 2, 5, 7-10], the spin frustration, quantum Rabi oscillations [2], quantum magnetization, owing to the spin-frustrated doublets and tunneling gap at level crossing (LC) field [14-21, 7-10] anisotropy of magnetization [13-24], anisotropy of EPR spectra [13, 9, 10, 18, 25, 27, 30, 31] and inelastic neutron scattering (INS) spectra. [29, 34, 35], field dependent spin chirality [30-33] and spin reorientation [32, 33] in the antiferromagnetic (AFM) $V_3$ [7,8], $\{\text{Cu}_3\}$ [9, 10] molecular magnets, and $V_3$ ring of $V_{15}$ single-molecular magnet (SMM) [14-31]. The single peak of the differential magnetization at LC field observed in $V_3$ [7] shows that the ground branch of $V_3$ possesses the avoided LC structure and large tunneling gap $\Delta_J$ at LC field [7, 8]. The quantum magnetization at LC field in the $V_3$ ring of $V_{15}$ [14-17] and $V_3$ [7, 8], $\{\text{Cu}_3\}$ [9, 10] nanomagnets was explained by the action of the in-plane and out-of-plane DM exchange coupling, different mixing of the spin-frustrated states characterized by the different spin chirality with the $S=3/2$ state, and tunneling gap $\Delta_J$ at LC. The spin chirality of the trinuclear nanomagnets has been proposed [3, 5, 7, 9, 10, 36-38] as the parameter for electric control of the spin triangles as units for molecule-based devices.

In multiferroics, electric polarization $\mathbf{P}$ can be significantly modified by the application of a magnetic field [39-52], the magnetic-field induced generation or flop of $\mathbf{P}$ show strong magnetoelectric coupling (for review see Refs [44, 45]). The spin current model of Katsura, Nagaosa and Balatsky (KNB) [39] or inverse DM model [40, 41] of the polarization $\mathbf{P}$ in multiferroics proposed that the neighboring canted spins ($\mathbf{S}_i$ and $\mathbf{S}_j$) produce the electric polarization $\mathbf{P} = \sum_{ij} A_{ij} [\mathbf{e}_{ij} \times [\mathbf{S}_i \times \mathbf{S}_j]]$, where $\mathbf{e}_{ij}$ is the unit vector connecting the sites $i$ and $j$. Microscopic expressions for the $A_{ij}$ constant, which depend on the superexchange and SOC, were obtained in [42, 43], $A \sim 10^{-10} \mu C / m^2$. The existence of the DM exchange is an essential ingredient in the theory [39-43] of the magnetoelectric effect in multiferroics with noncollinear spins. The exchange-striction mechanism of $\mathbf{P}$ was also proposed [51, 52, 42b] for the explanation of $\mathbf{P}$ in some collinear AF. Direct evidence of the spin current mechanism and the key role of the vector chirality $\kappa$ have been confirmed in multiferroics with the spiral spin structures [44, 45]. The investigations of $\mathbf{P}$ in multiferroics in transverse and tilted magnetic field [46-50] show important role of the magnetic anisotropy in the $\mathbf{B}$ induced polarization.

The DM induced multiferroic behavior in tetramer SMM with the polarization $\mathbf{P}$ in the KNB model in the form of the sharp peaks at the level crossing has been predicted first in Ref [53]. The spin-electric coupling in the $\{\text{Cu}_3\}$ nanomagnet, originating from a modified exchange constants induced by the applied electric field, was proposed recently [37, 38]. Since the spiral-spin magnets are potential candidates of the new multiferroic materials [54] the systems with the toroidal magnetic moment $\mathbf{T} = \frac{1}{2} \mu_0 g \sum [r_i \times \mathbf{S}_i]$ of the spins with the circular arrangement also attract attention [54-59]. In the trinuclear SMM, the Jahn-Teller effect [57] and the local magnetic anisotropy [59] result in $\mathbf{T}$ which interact with electric field. The polarization in the KNB model, toroidal moments, spin chirality and spin canting in the V3 DM nanomagnet in the applied magnetic field $B_z \parallel Z$ (along the trigonal axis Z) have been investigated in Refs [32, 33]. The DM $V_3$ analog of
multiferroics demonstrates the field induced \( \mathbf{P} \) and \( \mathbf{T} \), non-linear field dependence of the spin chirality and complicated spin dynamics at the avoided LC[32, 33].

The KNB polarization \( \mathbf{P} \) and toroidal moment \( \mathbf{T} \) of \( V_3 \), induced by the in-plane DM coupling, as well as their correlations with the spin chirality, spin fluctuations and canting and magnetic moment \( \boldsymbol{\mu} \) have not been considered in transverse field \( \mathbf{B}_z \). Since \( \mathbf{P} \) in multiferroics strongly depend on the orientation and tilt of the applied magnetic field \( \mathbf{B} \), it is essential to consider the polarization of DM \( V_3 \) analog of multiferroics in transverse field. Field dependence of the spin chirality and spin canting, the spin dynamics at the avoided level crossing and the microscopic mechanisms of the energy-levels repulsion also have not been considered for \( V_3 \) in transverse field \( \mathbf{B} \perp \mathbf{Z} \). Because the avoided LC has different structure in the field \( \mathbf{B}_z \perp \mathbf{Z} \) directed in the triangle plane and perpendicular to the triangle plane \( \mathbf{B}_z \parallel \mathbf{Z} \) it is necessary to investigate the field-induced spin dynamics at the avoided LC states in \( \mathbf{B}_z \), the microscopic origin of the field-induced spin canting and fluctuations in transverse field, and their correlations with \( \mathbf{P}, \mathbf{T}, \boldsymbol{\mu} \) and chirality. The consideration of the avoided LC is of interest because this magnetic repulsion of the Zeeman levels determines the magnetic and spectroscopic LC characteristics of the DM metal trimers [7-10, 16-33], metal rings [60] and the quantum superposition of states with different spin length [61] at LC in SMM. The joint consideration of the DM induced KNB polarization \( \mathbf{P} \), spatial spin canting and fluctuations, spin chirality \( \kappa, \chi \), toroidal \( \mathbf{T} \) and magnetic \( \boldsymbol{\mu} \) moments, their response to transverse and tilted magnetic field \( \mathbf{B} \), spin dynamics at the avoided LC is important for potential use of these characteristics in molecular-based devices. The purposes of this paper are i) to consider the KNB polarization \( \mathbf{P} \) of \( V_3 \) DM nanomagnet in transverse field \( \mathbf{B}_z \); ii) to investigate the spin dynamics (field-induced spin canting) generated by DM exchange at the ground and excited states of the avoided LC structures with tunneling gap \( \Delta_3 \) at LC in transverse field \( \mathbf{B}_z \) and correlations of the spin canting with \( \mathbf{P}, \mathbf{T} \) and chirality in this case; 3) to consider the dependence of the vector \( \kappa \) spin chirality on transverse magnetic field \( \mathbf{B}_z \) and correlations between the vector chirality \( \kappa \) and the spin canting and the spin structures, \( \mathbf{P}, \mathbf{T} \) and \( \boldsymbol{\mu} \) in \( \mathbf{B}_z \); 4) to investigate the DM induced toroidal moment \( \mathbf{T} \) in transverse field and its correlations with the spin fluctuations and the in-plane spin canting.

### 2. DM model of \( V_3 \) trimer with DM(x) mixing in transverse field

The exchange Hamiltonian of EQ V3

\[
H = \sum_{ij}(J\mathbf{S}_i \cdot \mathbf{S}_j + \mu_{\text{eff}} g_i \mu_i \mathbf{S}_i \cdot \mathbf{B}) + H_{\text{DM}} + D_{\text{ax}}[S_x^2 - S_y(S+1)],
\]

(1)

includes the Heisenberg isotropic exchange, the antisymmetric DM Hamiltonian \( H_{\text{DM}} \)

\[
H_{\text{DM}} = D_{\text{ax}} \sum_{ij} \{ [S_x \times S_y]_x + D_x \{ [S_x \times S_y]_y - \frac{1}{2}[S_x \times S_z]_z - \frac{1}{2}[S_z \times S_y]_y + \frac{\sqrt{6}}{2}[S_z \times S_x]_x + \frac{\sqrt{3}}{2}[S_z \times S_x]_x \}
\]

\[
- \frac{\sqrt{6}}{2}[S_z \times S_x]_x + D_x \{ [S_x \times S_y]_y - \frac{1}{2}[S_x \times S_z]_z - \frac{1}{2}[S_z \times S_y]_y - \frac{\sqrt{6}}{2}[S_z \times S_x]_x + \frac{\sqrt{3}}{2}[S_z \times S_x]_x \},
\]

(2)

in the right-handed (XYZ) cluster, and the \( S = 3/2 \) ZFS term where \( D_{\text{ax}} \) is the axial ZFS parameter, \( ij = 12, 23, 31 \). The pair out-of-plane \( D_x \) vector components \( (D_x = D^*_{y}) \) are oriented along the Z-axis perpendicular to the triangle \( XY \) plane. The pair in-plane \( D_x \)
DM interaction \((D_x = D_y)\) is lying in the triangle plane bisecting the \(ij\) bonds between the \(ij\) sites, the pair \(D_y = D_{ij}^y\) DM interactions are parallel to the \(ij\) bonds. The energy-level scheme of the \(S_z = 1/2\) trimer with the DM mixing in transverse field \(B \perp Z\) has been considered [7-10, 16, 17, 22-25, 28-32], however, the dependence of the states and LC on the spin chirality in transverse field, the correlations between the levels, avoided LC structure and the spin canting, chirality, fluctuations, polarization \(P\) and toroidal \(T\) and magnetic moments in \(B \perp Z\) were not considered.

In Fig. 1 for \(V_{3x}^R\) with \(D_z < 0\) and the \(D_x\) coupling, we show the scheme of the spin levels, spin chirality and tunneling gaps in transverse field \(B_x \perp Z\) of \(V_{3x}^R\) with

\[
\chi(B_x) = 0
\]

GS of the right zero-field (ZF) vector chirality \(\kappa_1^0 = \kappa_\parallel^0 = +1\), \(J = 4.8\, \text{K}\), \(D_z = D_x = -0.5\, \text{K}\), \(D_y = 0\), \(g = 1.95\), \(2D_0 = -0.120\, \text{K}\) [7, 8]. The ZFS of the spin-frustrated \(2(S = 1/2)\) set is formed by the \(D_z\) -coupling with the small in-plane \(D_p\) admixture of the \(S = 3/2\) states [23, 24, 28, 29]. The magnetic and spectral behavior in the vicinity of LC \(B_{AC} = -B_{AC}\) is determined by the three level schemes, which consists of the I–III avoided LC structure, and the linear ES II without the DM mixing with the \(|3/2, -3/2 >_x\) in Fig. 2. The GS I {the second ES III } of the avoided LC structure with tunneling gap \(\Delta_{\text{in}}\) at \(B_{AC} = B_{AC}\) field demonstrates the field-induced \([S_{gr} = 1/2 \rightarrow S_{gr} = 3/2]\) \{\([S_{ex} = 3/2 \rightarrow S_{ex} = 1/2]\)\} spin transition. The \(D_x\) induced tunneling gap \(\Delta_{\text{ex}}\) between the states I and III in transverse field at the avoided LC field \(B_{AC}\) is \(\sqrt{2}\) smaller than gap \(\Delta_{\text{in}}\) in the field \(B||Z\), \(\Delta_{\text{ex}} = 0.530\, \text{K}\) in Fig. 1. The change of the positive chirality \(\kappa_1, \kappa_\parallel\) of the lowest \(1^R_x\) \{\(\phi_{\text{ex}}^R(S_{12} = 1)\) and

Fig. 1. Energy level scheme of the \(V_{3x}^R\) trimer with the in-plane \(D_x\) spin mixing in transverse magnetic field \(B_x \perp Z\).
II^R_x [ \Phi^R_{\text{I}}(S_{12} = 0) ] states in an increasing field B_x is presented in Fig. 1. The scheme of the spin levels of V_{3x} trimer with D_z > 0 has the form of Fig. 1 with the ground \Gamma^L_x, \Pi^L_x doublet, characterized by the negative ZF (0T) vector chirality \kappa^0_1 = \kappa^0_\Pi = -1. The spin chirality in transverse field is considered in Sec. 4, 5.

In the H_{\text{DM}} model (D_x = D_y = 0), the ground double-degenerate I,II doublet exhibits simple crossing with the \{3/2, -3/2, >_z \} state at LC field B_{AC}, Appendix A. The wavefunctions \Phi^0_{\text{I}}, \Phi^0_{\text{II}} of the degenerate GS (1,II) of the 2(S=1/2)_x sector the H_{\text{DM}} model in B_x are given in Appendix A in the representations of the chirality and intermediate spin S_{12} quantum numbers. The D_x coupling splits the double-degenerate (\Phi^0_{\text{I}}, \Phi^0_{\text{II}}) doublet of the H_{\text{DM}} model in B_x on the GS \Phi^0_{\text{I}}(S_{12} = 1) and ES \Phi^0_{\text{II}}(S_{12} = 0) characterized by S_{12} = 1 and S_{12} = 0, respectively, Fig. 1.

3. Polarization of V_3 with DM(x) mixing in transverse field B \perp Z

The KNB polarization operator P of the spin current model [39] for multiferroics has the form

\[ P = \sum_q A_q [e_q \times (S_i \times S_j)], \]  

(3)

where \( e_q \) is the unit vector connecting the sites i and j. This KNB operator for the V_3 DM system (A_q = A) can be represented [31, 32] in the form

\[ P = P_z + P_x + P_y, \]

where

\[ \begin{align*}
P_z &= -e_z A [S_1 \times S_2]_x - [S_2 \times S_3]_x - [S_3 \times S_1]_x + \sqrt{2} \left( [S_2 \times S_3]_y - [S_1 \times S_3]_y \right), \\
P_x &= -e_x (A/2)(2[S_1 \times S_2]_z - [S_2 \times S_3]_z - [S_3 \times S_1]_z), \\
P_y &= e_y (A \sqrt{2} / 2) ([S_2 \times S_3]_z - [S_1 \times S_3]_z) 
\end{align*} \]

in the right-handed cluster frame, \( e \) is the unit vector. The P_3 spin part of the polarization operator \( P_z = -e_z A P_3 \) (4) coincides with the spin operator of the in-plane H_{\text{DM}}(x) coupling in Eq (3) \( P_1 = H_{\text{DM}}(x)/D_z \) (\( D_z = 1, D_z = D_y = 0 \)). In the H_{\text{DM}} model \( (D_p = 0) \), the KNB polarization is equal to zero, \( P_{\text{KNB}} = 0 \).

In transverse field B_x \perp Z, the D_z coupling (Fig. 1) determines the KNB P and spin canting of V_{3x}. In Fig. 2, we depict polarization P_{\text{N}}(B_x) || Z numerically calculated in the KNB model (4) for GS N = I and ES II, III of Fig. 1. \( D_z = D_x = \pm 0.5K \), \( J = 4.8K, D_y = 0 \). The superscripts +(-) or L(R) in P_{\text{N}}(\pm) (B_x) = P_{\text{N}}^{(R)(L)} correspond to \( D_z = D_x = (+(-)0.5K \) of V_{3x} (V_{3x}). In increasing B_x, the KNB P_1 (solid curve in Fig. 2) of the GS I^L_x (\( \kappa^1_1(0T) = 1 \)) of V_x increases non-linearly from the ZF value \( P_{10} \), shows the maximum \( P_{1}^{(R)}(\text{max}) = 0.526A \) at \( B_{AC} \), and, then, decreases slowly for \( B_x > B_{AC} \). The total increase is \( \Delta P_{1}^{(R)}/P_{10} \approx 6 \), \( \Delta P_{1}^{(R)} = P_{1}^{(R)}(\text{max}) - P_{10} \). P_1 (dash) of GS II^L_x (\( \kappa^1_1(0T) = -1 \)) of V_{3x} shows the similar non-linear increase from the ZF \( P_{10} \) to the \( P_{1}^{(R)}(\text{max}) = 0.532A \) at \( B_{AC} \), and, then, decrease for \( B_x > B_{AC} \), \( \Delta P_{1}^{(R)}/P_{10} \); 22, Fig. 2.
The KNB polarization $P^R_N (P^L_N)$ of the lowest levels of $V^R_{3x} (V^L_{3x})$ in transverse field $B_x$.

The KNB $P^{R(L)}_N (B_x)$ does not change the direction with sweeping $B_x$ along the X-axis: $P^{R(L)}_N (B_x) = P^{R(L)}_N (B_x)$, (see Fig. 6b). For $|B_x| > 3T$, the values of $P^R_1$ and $P^L_1$ are very close and does not depend practically on the signs of the chirality: $|P^L_1| \approx |P^R_1|$, Fig. 2. At the same time, the LFP$^R_1$ and $P^L_1$ differ significantly, Fig. 2. The ZF $P^{R(L)}_{I,0} = P^{R(L)}_{II,0}$, $P^{R(L)}_{III,0} = P^{R(L)}_{IV,0}$ for $B_x \perp Z$ coincide with that for $B_z \parallel Z$ [31, 32].

$P^R_1$ of the first linear ES $II^R_1$ (Fig. 1), is very small (Fig. 2, $P^L_1 = |P^R_1| = P^L_1$ for $|B_x| > 3T$) and does not depend on $B_x$. $P^R_{III} (P^R_{III})$ of the ES III is opposite in the sign to $P^R_1$ ($P^L_1$) and practically coincides with $P^L_{III} (P^R_{III})$ for $|B_x| > 3T$ in Fig. 2.

4. Spin canting and spin chirality in transverse field in the $H_{DM}^z$ model

A. Spin canting in the DM(z) model without the $D_z$ spin mixing

The vector chirality is a key factor for the appearance of polarization in multiferroics [44, 45]. The spin chirality and canting in the field $B_z \parallel Z$ were considered in [31, 32]. Only zero-field spin chirality of the trimers with strong Heisenberg exchange is usually considered and only one type of chirality (or vector, or scalar chirality) is discussed. For better understanding the role of the chirality and spin canting in polarization $P$ in transverse field $B_x$ we consider first these characteristics of $V_3$ in the $H_{DM}^z$ model with $D_\perp = 0$. In Fig. 3a for $V^R_{3x} (D_z < 0)$ in the $H_{DM}^z$ model in $B_x$, we depict field dependence of the $m_iz, m_iz, m_iz, m_iz, m_iz, m_iz$ projections of the spins $\mathbf{S}_i$ and $\mathbf{S}_i$ in the XY plane in the $I_1$ and $I_2$ lowest double-degenerate $\Phi_1^0 = \Phi_1^0, \Phi_1^0 = \Phi_1^0$ states which coincide with the level II in Fig. 1. The out-of-plane
$m_i$ projections in $B_x$ are equal to zero in the $\mathbf{H}_{\text{DM}}'$ model, $m_x = m_{ix} = 0$, and the individual spins $\mathbf{S}_i = \mathbf{S}$ and $\mathbf{S}_i = \mathbf{S}_i$ lie in the $XY$ plane, as shown in the planar schemes in Fig. 3a, where the arrows at the vertices schematize the $m_{ip} = \mathbf{S}_i$ (Schemes $Ia$, $Ib$) and $m_{ip} = \mathbf{S}_i$ (IIa) in-plane spin projections. In the low field (LF) $B_x = +2mT$, all the in-plane $m_{ip}$ projections have the same value in the Schemes $Ia$ and IIa for in the I and II ([$m_{ip} | m_{ip}_i$] = 1/3, $i = 1, 2, 3$). In the LF planar 120° spin structure $Ia$ (IIa) in Figs. 3a, 3b, the $\mathbf{S}_i$, ($m_{ip}$) $\mathbf{S}_i$ arrows point directly towards [away from] the triangle center. An increasing field ($B_x > 1.5T$) results in the high-field (HF) constant values $m_{3x} = 1/6$ and $m_{3x} = -1/2$ for I and II, respectively, in Fig. 3a. The in-plane $|m_{ip}| = |m_{ip}|$ of $I_{R}$ (Fig. 3a) show very weak field dependence at LF, $|m_{ip}| = |m_{ip}| = 1/3$ for $B_x > 1T$, while for II $|m_{ip}| = |m_{ip}| = 0$, $|m_{ix}| = |m_{ix}| = 0$ for $B_x > 2T$. The $m_{ip}$ have opposite signs for $B_x > 0$ and $B_x < 0$ in Fig. 3. Small negative field ($B_x = -2mT$) changes the in-plane orientations of the spins and results in the 120° spin structure $Ib$ for $I_{R}$. The in-plane GS spin structure at HF $B_x$ ($B_x > B_{AC}$) shows the collinear $S = 3/2$ spin Scheme $I\alpha$ ($M_x = -3/2$, $m_{ix} = -1/2$) for $B_x > 0$ and $I\beta$ ($M_x = 3/2$, $m_{ix} = 1/2$) for $B_x < 0$ in Fig. 3a. The $B_x$ variation of a net in-plane projections $M_{ix} = M_{ix}$ of the total spins $\mathbf{S}_i$ and $\mathbf{S}_i$ of the I and II states $M_{ix} = M_{ix} = -h_{ij} / \sqrt{3D_2^2 + 4h_{ij}^2}$, describes the non-linear change of $M_x$ from the zero ZF $M_x^0(0T) = 0$ to the value $M_x = 1/2$ ($M_x = 1/2$) at positive (negative) HF $B_x$ before LC. $P = 0, T = 0$ for all the states and spin structures in Fig. 3 of the $\mathbf{H}_{\text{DM}}'$ model in field $B_x$.

An increase of the field $B_x \parallel X$ reduces the symmetry from the trigonal $C_3$ to the rhombic $C_2$, forms the intermediate $S_{12}$ spin of the states and changes the LF spin structures a) and b) of Fig 3a in the $\mathbf{H}_{\text{DM}}'$ model. Fig. 3b shows the field-induced transformation of the LF in-plane $Ia$ and IIa spin-frustrated 120°-spin structures into the HF planar $S = 1/2$ spin configurations, which are characterized by $S_{12} = 1$ ($m_{ix} = m_{ix} = -1/3, m_{ix} = 1/6$ for HF $B_x$, $m_{iy} = 0$) and $S_{12} = 0$ ($m_{ix} = m_{ix} = 0, m_{3x} = -1/2$ for HF $B_x$, $m_{iy} = 0$), respectively, $m_i = |m_{ip}| = |m_{2p}|$, $m_1 = |m_{ip}| = |m_2| = |m_{2p}|$ in Figs. 3b, 3c. Fig. 3b also shows the projections $M_{ix}$ of $\mathbf{S}_i$ and corresponding vector chirality $\kappa_{1}^{R,L}$, $\kappa_{II}^{R,L}$ of the $I^{R,L}$ and $II^{R,L}$ states of the $\mathbf{H}_{\text{DM}}'$ model; $M_{ix} = 0$. The superscripts $R(L)$ or $(-+)$ correspond to $D = D_{x} = -(+0.5K)$. For $V_{3}^{R}$, the LF 120° planar structure $Ia$ of the $I^{R}$ state with the LF maximum $\kappa_{1}^{R}(2mT) = 1$. $M_{ix} \approx 0$ is transformed at HF $B_x = 4T$ into the $Ic$, which is very close to
Fig. 3 The in-plane spin structures of the I and II levels of the double-degenerate lowest (\(\Theta_{I_x}^0, \Theta_{II_x}^0\)) state of \(V_3^R\) in the \(H_{DM}^z\) model (\(D_p = 0\)) in transverse field \(B_x \perp Z\). The out-of-plane \(m_{ix}\) spin projections are equal to zero. a) The in-plane spin projections \(m_{in}\) (\(m_{in}^\perp\)) of the state I (II), the low-field 120° (Ia, IIa for \(B_x > 0\) \(\text{and } B_x < 0\)) and high-field collinear (Iaβ, IIβ) spin structures for \(D_z, D_x < 0, D_y = 0\). The field variation of the in-plane spin structures of the states of \(V_3\) in the \(H_{DM}(z)\) model with \(D_z, D_x < 0\) (I, II) and \(D_z, D_x > 0\) (Γ, II′) in magnetic field \(B_x \parallel X\) (b) and \(B_y \parallel Y\) (c).
the spin-collinear HF $|S = 1/2, S_{12} = 1 >_x$ structure, $[\kappa^R_1(4T) = +0.16, \ M_{ix} = -0.494, \ \mu_{ix} = 0.99 \mu_B]$. This $\Phi_{ix}(S_{12} = 1)$ is mixed with the $[3/2, -3/2 >_x$ in Fig. 1. The LF IIa(2 mT) in-plane 120°-structure of II$^R$ with $\kappa^R_{II}(2 mT) = +1$ is transformed at HF into the planar IIc, which is very close to the HF $|S = 1/2, S_{12} = 0 >_x$ spin structure $[\kappa^R_{II}(4T) = +0.16, \ M_{ix} = -0.494]$, Fig. 3b.

The Schemes I’ and II’ in Fig. 3b show the field induced change of the in-plane structures of the two spin-frustrated I$^L$, II$^L$ states of V$^L_3$ in the $\textbf{H}_{dm}^y$. The LF (2 mT) 120° spin structure Ia’ of I$^L$ with maximum LF $\kappa^L_1 = -1$ ($M^*_x \approx 0$), is transformed at $B_x = 4T$ into the in-plane HF $|1/2, S_{12} = 1 >_x$ structure Ic’ $[\kappa^L_1(4T) = -0.16, \ M^*_x = -0.494]$. The LF spin structure IIa’(2 mT) ($\kappa^L_{II} = -1$) tends into the HF in-plane $|1/2, S_{12} = 0 >_x$ spin structure IIc’ ($\kappa^L_{II}(4T) = -0.16$).

The in-plane spin structures of the $\textbf{H}_{dm}^y$ model also depend on the orientation of the in-plane field $B_x$. Fig. 3c shows the in-plane spin structures, the local spin projections, spin chirality and the values $M_y$ of the total spin projections of the system of Fig. 3b in the external in-plane magnetic field oriented parallel to the $Y$-axis, $B_y \parallel Y$. The in-plane spin structures I, II $\{I’, II’\}$ of the states of the positive vector chirality, $\kappa^R_1(B_y)$, $\kappa^R_{II}(B_y) > 0$ {negative chirality, $\kappa^L_1(B_y)$, $\kappa^L_{II}(B_y) < 0$} differ from the corresponding in-plane spin structures in Fig. 3b for $B_x \parallel X$ by the $\pi/2$-rotations of the corresponding individuals spin $S_i$ arrows at the $i$-vertexes. At the same time, the dependence of the vector chirality $\kappa^R_{1(II)}(B_y)$ is the same for $B_x \parallel X$ and $B_y \parallel Y$. 

125
B. Spin Chirality in $H^{\text{DM}}$ model without DM(x) mixing

The operators of the vector spin chirality $\hat{K}_z$ [62] and the scalar spin chirality $\hat{C}$ [36,37] of the $S_z=1/2$ trimer system have the form

$$\hat{K}_z = (2/\sqrt{3})\left( [S_z \times S_x]_z + [S_z \times S_y]_z + [S_z \times S_x]_z \right),$$

$$\hat{C} = (4/\sqrt{3})S_z \cdot [S_z \times S_x].$$

The DM $D_z$ exchange determines the vector $\kappa$ and scalar $\chi$ spin chirality of $V_3$ in magnetic field $B_z \parallel Z$ [30-32]. The in-plane components of the chirality vector are equal to zero in the ground and excited states of $V_{3x}^R, V_{3x}^L$ for $B_z \parallel Z$ and $B_z \parallel X$, $\kappa_x = <\hat{K}_x> = 0$, $\kappa_y = <\hat{K}_y> = 0$.

The GS scalar $\chi$ chirality in the field $B_z \parallel Z$ correlates with the vector chirality $\chi_1^+(B_z) = -\kappa_1^x$ for $B_z > 0$, $\chi_1^+(B_z) = \kappa_1^y$ for $B_z < 0$ [32]. The scalar chirality $\chi_N(B_z) = <\Phi_{R(L)}^{\text{tr}} | \hat{C} | \Phi_{R(L)}^{\text{tr}} >$ in transverse field $B_x \perp Z$ is equal to zero, $\chi_N(B_z) = 0$.

In Fig. 4a ($B_z > 0$), we plot calculated right {left} vector chirality $\kappa_1^R = \kappa_1^L(B_z)$ for the GS $\Gamma \{ \Gamma = \Gamma' \}$ with $S_{12} = 1$ of $V_{3x}^R \{ V_{3x}^L \}$ in the $H^{\text{DM}}$, $\kappa_{1R}^{\text{tr}} = <\Phi_{R(L)}^{\text{tr}} | \hat{K}_z | \Phi_{R(L)}^{\text{tr}} >$, and $\kappa_1^R = 1$ $[\Delta_1^- = -1]$ of $V_{3x}^R \{ V_{3x}^L \}$ in $B_z \parallel Z$. Fig. 4a also shows the in-plane $m_3$, $m_y$, $m_2y$ projections, the in-plane spin structures, $\kappa_{1R}^{\text{tr}}$, and canting angles $\zeta$ for $S_1, S_2, S_3$ in the GS $\Gamma$ and $\Gamma'$ of Fig. 3b. The chirality $\kappa_{1R}^{\text{tr}}(B_z)$ strongly decreases non-linearly with an increase of $B_z$. The in-plane canting angle $\zeta(B_z) = \zeta_x$ for $S_1 (m_1 = m_{ip}) \{ S_2 (m_2 = m_{ip}) \}$ in Fig. 4a for the $S_{12} = 1$ GS is determined by equation

$$\tan \zeta = \Delta_0 \sqrt{3} / (\epsilon_x^0 + h_x),$$

(7)

$\zeta(B_z)$ is the angle between the resulting in-plane $m_{ip}$ projections and the X axis, ($i = 1,2$) Fig. 3a. The initial LF canting angle is $\zeta_0(B_z = 2 \text{mT}) = \pi / 3$ for $S_1, S_2$ and all initial LF radial $m_{ip}$ projections (arrows) have the same value (length) $|m_{ip}^R| = 1/3$ in Figs. 3a, 3b. The increasing $B_z$ rotates the $m_3, m_y$ arrows of the nearly constant length at the 1 and 2 vertices in the triangle plane in the opposite directions, Fig. 4a. The HF $B_x$ orients the $m_{ip}$ and $m_{ip}$ projections parallel to the X axis, $\zeta \rightarrow 0$ at HF in Eq. (7), Figs. 3b ($\Gamma c, \Gamma c'$) and 4a. At the same time, the increasing $B_z$ simultaneously changes only the length of $m_3 (m_{3x} = 1/3 \rightarrow m_{3x} = 1/6 )$, $m_{ip} \parallel B_z$. This field-induced in-plane $[\zeta_1, m_1; \zeta_2, m_2; m_3] = [\zeta, m_{ip}]$ spin-canting tends to the collinear HF $|S = 1/2, S_{12} = 1 > \chi$ spin structure in Figs. 3b and 4a. The in-plane canting angle $\zeta'' = \zeta_{1L}$ for the $S_1, S_2$ spins with the decreasing length $m_{ip} = m_{2p}$ (Fig. 3a) of the $\Gamma$ and $\Gamma'$ states with $S_{12} = 0$ (Fig. 3b), is determined by equation $\tan \zeta'' = \Delta_0 \sqrt{3} / (\epsilon_x^0 - h_x)$.

The field dependence of the vector chirality $\kappa_{1R}^{\text{tr}}(B_z)$ (Fig. 4a) has the form

$$\kappa_{1R}^{\text{tr}}(B_z) = +(-) |D_z| \sqrt{3} / \sqrt{3D_z^2 + 4h_x^2} = +(-) 2\sqrt{3} |m_{ip}| = +(-) 2\sqrt{3} |m_{ip}| \sin \zeta_{1L},$$

(8)

126
in the $H_{\text{DM}}^x$ model, \( \sin \zeta_x = \Delta_0 \left\{ 3 / [ (\epsilon_x^0 + h_x)^2 + 3\Delta_x^2] \right\}^{1/2} \), \( B_x > 0 \). The \( \kappa_{\text{III}}^{R(L)}(B_x) \) is determined by the out-of-plane \( D_z \) coupling and \( B_x \), \( \kappa_{\text{II}}(B_x) \| Z \), \( \kappa_{\text{I}}^{R(L)} = \kappa_{\text{III}}^{R(L)} \). The field-dependent vector chirality \( \kappa_{\text{II}}(B_x) \propto m_{ly} \) (Eq. (8)) correlates with the \( D_z \)-induced in-plane spin fluctuations \( m_{ly}, m_{zy} \) of the \( S_1, S_2 \) spins ( \( m_{zy} = -m_{ly} \)). Since the in-plane \( m_i = |m_{ip}| = m_{iz} = |m_{zp}| \) are changed very slowly only at LF (Figs. 3a and 4a), the GS \( \kappa_{\text{I}}^{R} \) (8) \( [\kappa_{\text{I}}^{R}] \) directly correlates also with the in-plane spin canting \( \sin \zeta \) of the \( S_1, S_2 \) spins in Fig. 4a. The upper part of Fig. 4a for GS $1^R$

\[
\sin \zeta = \Delta_0 \left\{ 3 / [ (\epsilon_x^0 + h_x)^2 + 3\Delta_x^2] \right\}^{1/2} \]

\[
\kappa_{\text{I}}^{R(L)}(B_x) \propto m_{ly}
\]

\[
\kappa_{\text{II}}(B_x) \| Z
\]

\[
\kappa_{\text{III}}^{R(L)} = \kappa_{\text{IV}}^{R(L)} = -\kappa_{\text{I}}^{R(L)}
\]

Fig. 4a

Fig. 4a: The correlation between the vector spin chirality \( \kappa_{\text{I}}^{R(L)}(B_x) \) of GS of \( V_3^L \) (\( V_3^R \)) and the angle \( \zeta \) of the in-plane spin canting of the \( S_1 \) and \( S_2 \) spins in transverse field \( B_x \) in the $H_{\text{DM}}^x$ model. The low-field \( 120^\circ \) spin structures with \( \kappa_{\text{I}}^{m} = \pm 1 \) correspond to \( \zeta_0 = 60^\circ \). b)

Fig. 4b

Fig. 4b: Coefficients \( n_1, n_2 \) and vector chirality \( \kappa_{\text{I}}^{R(L)}(B_x) \) of GS of \( V_3^L \) (\( V_3^R \)).
The field dependence of the contributions of the spin structures with positive ($\kappa_1 = 1$) and negative ($\kappa_1 = -1$) vector chirality to a net GS spin chirality and simultaneous variation of the $S_{\perp}$-structures contributions to GS in transverse field $B_z$.

of $V_3^R$ shows that the positive GS $\kappa_1^R(B_z) \propto \sin \zeta$ describes the in-plane anticlockwise and clockwise rotations of the $S_1$ ($m_1$) and $S_2$ ($m_2$), respectively in the increasing $B_z$. Eq. (8) and Fig. 4a explain the correlations between the vector chirality $\kappa_1^R(B_z)$ and the spin structures in the planar Schemes $Ia$, $Ib$, and $Ic$ in Fig.3b. In the field-induced $[\zeta, m_i]$ spin-canting in $H_{DM}$, the $S_1$ and $S_2$ spins rotate in the $V_3^R$ plane, beginning from an initial internal canting angle $\zeta_0 = \pi / 3$ in the LF planar 120$^\circ$ spin scheme $I_a^R$ with the radial $|m_i| = 1/3$ arrows and $\kappa_1^R(0T) = 1$, to the HF $\zeta = 0$, which corresponds to $\kappa_1 \to 0$ and the collinear planar HF $|1/2, S_{\perp}| = 1 >_x$ configuration with $m_{ix,ix} \to -1/3$, $m_{3x} \to 1/6$, $M_{ix} = \sum m_{ix} \to -1/2$. For the lower $V_3^L$ part of Fig. 4a, the negative vector chirality $\kappa_1^L(B_z) \propto -\sin \zeta$ of the GS $I_a$ describes the clockwise and anticlockwise in-plane $\zeta$-rotations of the $S_1$ ($m_1$) and $S_2$ ($m_2$), respectively, in the opposite directions in the spin schemes for $\kappa_1^L < 0$. The field-induced in-plane $[\zeta, m_i]$ spin-canting for $V_3^L$ represents the transformation from the LF (2mT) planar 120$^\circ$ spin structure $I_a^L$ [with the LF $|m_i| = 1/3$, the external ZF in-plane canting angle $\zeta = 60^\circ$ for the $S_1$, $S_2$ and $\kappa_1^L(0T) = -1$[Figs. 4a and 3b, $I_a^L$] to the collinear HF $|S = 1/2, S_{\perp}| = 1 >_x$ spin structure with $m_{ix} = m_{2x} \to -1/3$, $m_{3x} \to 1/6$, $\zeta \to 0$, $\kappa_1^L \to 0$. The $\kappa_1^L < 0$ spin Schemes in Fig. 4a and the $\kappa_1^L(B_z)$ curve explain the correlations between the vector chirality $\kappa_1^L(B_z)$ and the in-plane spin structures in the planar Schemes $Ia'$, $Ib'$, and $Ic'$ for $I_a^L$ of $V_3^L$ in Fig.3b.

In the DM metal trimers on a two-dimensional AFM frustrated kagome lattice, the spin chirality is correlated with the spin canting in the in-plane ZF spin structures [63-65]: the 120$^\circ$ in-plane $q = 0$ spin structures in Fig. 2b in [63] ($D_z < 0$, $D_p = 0$) for the neighboring triangles with the radial spin vectors (arrows) directed from and toward the center of the triangle possess positive (+) chirality [see the planar $Ia$ and $IIa$ structures in Fig. 3b]. The planar spin structures for the neighboring triangles in Fig. 2c [63] for $D_z > 0$, $D_p = 0$ possess negative (−) chirality [see the planar $Ia'$ and $IIa'$ structures in Fig. 3b]. The LF in-plane radial 120$^\circ$-spin structures $Ia$ and $IIa$ with the $|m_{ip}| = 1/3$ arrows in Fig. 3b of the magnetically isolated $V_3^R$ with the LF chirality $\kappa_1^R = 1$ in $B_x$ coincide in the form with the standard in-plane 120$^\circ$-spin $q = 0$ structures in Fig. 2b [63] for the neighboring triangles with the + chirality of a 2D frustrated AFM+DM kagome lattice ($D_z < 0$, $D_p = 0$). The LF in-plane 120$^\circ$-spin structures $Ia'$ and $IIa'$ with the same $|m_{ip}| = 1/3$ arrows (Fig. 3b) of the isolated $V_3^L$ with LF $\kappa_1^L = -1$ in the transverse $B_x$ coincide in the form with the in-plane 120$^\circ$-spin
structures in Fig. 2c [63] for the neighboring triangles with the negative (−) chirality of the AFM+DM kagome lattice.

The difference in the correlations between the planar spin structures and the vector chirality in the cases of the magnetically isolated $V_3^R$, $V_3^L$, $H_{DM}^z$ triangles in transverse fields $B_x$, $B_y$ (Figs.3-4) in comparison with that for the triangles [63] of the AFM+DM 2D kagome lattice is the following: i) the LF in-plane $120^\circ$-spin structures $Ia$ and $Ila$ [ $Ia'$ and $Ila'$ ] of Fig. 3b for maximum positive $\kappa_1^R = 1$ [negative $\kappa_1^L = -1$] are obtained only in the small positive or negative $B_x$, ii) the spin structures and the $\kappa_1^R$ [$\kappa_1^L$] field behavior are different in the field $B_x \perp Z$ and $\kappa_{R(L)}(B_z)$ in $B_z \parallel Z$, iii) the in-plane spin structures of $V_3^R$, $V_3^L$ significantly depend on the value, direction and sign of the applied transverse field $B_x$ and $B_y$ [the $[\zeta,m_y]$ spin-canting in Figs. 3b and 3c], and iv) the vector spin chirality $\kappa_{R(L)}^l$ $||Z$ is characterized not only by the sign (+ or −) but also by the $\kappa_1^R$ [$\kappa_1^L$] values, which correlate with the in-plane opposite spin fluctuations $m_{1y}$, $m_{2y}$ of the $S_1$, $S_2$ spins in the planar spin structures in Figs. 3a and 4a. The scalar chirality is equal to zero for the in-plane spin structures in Figs. 3-4 in transverse field, as in the case of the planar structures of the AFM kagome lattice [36].

Fig. 4b shows the joint change of the vector chirality $\kappa_1^R(B_x)$ and the $S_{12}$ contributions to the GS $1^R$ of $V_3^R$ in $B_x$ for the $H_{DM}^z$ model. The GS wavefunction $\Phi_0^x(B_x) = \Phi_1(S_{12} = 1)$ in Fig. 4b represents the mixture of the $\Omega_+ [\kappa_1^R(B_x) = 1]$ and $\Omega_- [\kappa_1^L(B_x) = -1]$ states, characterized by $\kappa_1^R = 1$ and $\kappa_1^L = -1$, and the corresponding LF in-plane $n_i(Ia)$ and $n_z(ia')$ structures in Fig. 3b, $\Phi_1(S_{12} = 1) = n_1\Omega_+(1) + n_2\Omega_-(1)$. The $\Omega_-(1)$ [ $\Omega_+(1)$ ] state of the right chirality dominates in the LF $\Phi_0^x$ [ $\Phi_0^l$ ] state and the LF 1. II HF states. In Fig 4b, the $\Phi_1(S_{12} \rightarrow I)$ wavefunction of $1^R$ is also shown also in the $S_{12}$ representation, $\Phi_1(S_{12} \rightarrow I) = C_i\Lambda_.(S_{12} = 1) + iC_2\Lambda_.(S_{12} = 0)$. The LF maximum $\kappa_1 = \kappa_\Omega = 1$ corresponds to the same contributions of the $\Lambda_.(S_{12})$ states with $S_{12} = 1$ and $S_{12} = 0$ to the GS $\Phi_0^x$, Fig. 4d ($\Phi_{l}$). The HF $B_x$ in Fig. 4b forms the state $1^R$ characterized by $S_{12} = 1$ [ $m_{1x} = m_{2x} = -1/3$, $m_{3x} = 1/6$ (Fig. 3b, Ic)], and the $1^R$ state with $S_{12} = 0$ [ $m_{3x} \rightarrow -1/2$ $m_{1y} = m_{2y} \rightarrow 0$ (Fig. 3b, IId)]. On the other hand, these pure Heisenberg states in HF $B_x$, characterized by $S_{12} = 1$ (and $S_{12} = 0$), correspond to $\kappa_{l,\Omega} = 0$. The GS vector chirality $\kappa_1^R(B_x) = n_1^2 - n_2^2 = 2|C_i||C_2| = |d_1|/\sqrt{d_1^2 + h_x^2}$ is reduced to zero $\kappa_1 \rightarrow 0$ at HF $B_x >> 2\Delta_{DM}$ in the $H_{DM}^z$ model, Figs. 4a and 4b, $\kappa_\Omega = \kappa_1$, 129
\( \kappa_{\text{III}} = \kappa_{\text{IV}} = -\kappa_1 \). At the intermediate fields, the \( I^R \) and \( II^R \) states are the mixture of the states characterized by \( S_{12} = 0 \) and \( S_{12} = 1 \) (and \( \kappa^R = 1 \) and \( \kappa^\perp = -1 \)).

5. Spin chirality and polarization of \( V_{3x}^{R(L)} \) with the \( D_x \) coupling in transverse magnetic field

The in-plane \( D_x \) spin-mixing in the GS \([\Phi_{1x}(S_{12} = 1)] \) of \( V_{3x}^{R(L)} \) in \( B_x \) (Fig. 1) determines the spin chirality, canting and KNB polarization \( \mathbf{P} \). In Fig. 5 \((B_x > 0)\), we depict the field-\( B_x \)-dependence of the vector chirality \( \kappa_{N}^{R(L)}(B_x) \) of the lowest \( N = I, II, III \) states (Fig. 1) of \( V_{3x}^{R(L)} \) with the \( D_x \) coupling in comparison with the GS \( \kappa_{Nz}^{R(L)}(B_x) \) in the field \( B_x \parallel Z \) and the KNB polarization \( P_{1}^{R(L)} = P_{1}^{R(L)}(B_x) \). There is no correlation between \( P_{N}^{\perp}(B_x) \) and zero scalar chirality \( \chi_{N}^{\perp}(B_x) = 0 \) in transverse \( B_x \perp Z \). Figure 5 shows the \( B_x \)-field dependence of the right (left) vector chirality \( \kappa_{1}^{R(L)}(B_x) [ \kappa_{1}^{L}(B_x) ] \) of GS \( I_{1x}^{R}[I_{1x}^{L}] \) and \( \kappa_{II}^{R}, \kappa_{III}^{R} [ \kappa_{II}^{L}, \kappa_{III}^{L} ] \) of the excited \( II_{x}^{R} \), \( III_{x}^{R} [ II_{x}^{L}, III_{x}^{L} ] \) states of \( V_{3x}^{R(L)} \) and the KNB polarization \( P_{1}^{R(L)} \) in transverse field \( B_x \).

![Graph showing vector chirality and polarization](image)

**Fig. 5** The vector chirality \( \kappa_{N}^{R(L)} \) of the lowest states of \( V_{3x}^{R(L)} \) and the KNB polarization \( P_{1}^{R(L)} \) in transverse field \( B_x \).

of \( V_{3x}^{R(L)} \) in Fig. 1. The GS vector chirality \( \kappa_{1}^{R(L)}(B_x) \) for \( 0 < B_x < 4T \) in Fig. 5 coincides with that in Fig. 4a of the \( H_{DM}^{x} \) model. For \( B_x > 4T \), the \( \kappa_{1}^{R(L)}(B_x) \) decreases to zero at avoided LC field \( B_{AC} \). At the same time, the chirality \( \kappa_{II}^{R(L)} \) of the first ES \( II_{x}^{R(L)} \) which does not exhibit the \( D_x \) spin-mixing (Fig.1), has the same field dependence (gradual decrease) in Fig. 5 as \( \kappa_{1}^{R(L)} = \kappa_{II}^{R(L)} \) in the \( H_{DM}^{x} \) model in Fig. 4a. Small increase of the GS \( P_{1}^{R(L)} \) for \( 0 < B_x < 4T \) is accompanied with the large decrease of \( \kappa_{1}^{R(L)} \) from the ZF maximum \( \kappa_{1}^{R(L)} = \pm 1 \) to \( \kappa_{1}^{R(L)}(4T) = +(-)0.16 \) in Fig. 5. At the same time, the change of
the small $\kappa_R^{RL}$ chirality at $B_{AC}$ is accompanied by maximum of the KNB $P_1^{RL}(B_x)$, Fig. 5, $\kappa_1^{RL} = +(-)0.06$ at $B_{AC}$. The field $B_x^\pm$ of The maximum KNB $P_1^{RL} |_{\text{max}}$ at $B_{AC}^\pm$ is accompanied by the maximum of differential chirality, $d\kappa_i / dB_x$ and magnetic moment $[d\mu^i / dB_x]$. There is no correlation between constant small $P_1^{RL}$ of $\Pi_x^{RL}$ (Fig. 2) and the chirality $\kappa_\Pi^{RL}$, which decreases smoothly from ZF $|\kappa_\Pi|$ $=$ 1 to HF $\kappa_\Pi = 0$, $|\kappa_\Pi| > |\kappa_1|$ for $B_x > B_{AC}^\pm$ in Fig. 5. The chirality $\kappa_\Pi^{RL}$ $[\kappa_\Pi^{RL}]$ of the S=3/2 state $V$ is equal to zero for $B_x < 5T$. Then, for $B_x > 5T$, $\kappa_\Pi^{RL}$ tends to $\kappa_\Pi^{RL}$ in Fig. 5, when $\kappa_1^{RL} \to 0$. Field dependences $P_1^{RL}(B_y)$ and $\kappa_1^{RL}(B_y)$ in $B_y \parallel Y$ have the same forms as that in Fig. 5 for $B_x \parallel X$ in spite of different in-plane spin structures in Figs. 3b, 3c (in-plane isotropy), $\chi(B_y) = 0$.

6. Spin canting and avoided level crossing in $V_3$ with DM(x) mixing in transverse magnetic field. A. Magnetic field $B \parallel X$

To establish relationships between the polarization, toroidal moment and the spin canting and fluctuations in transverse field, Fig. 6a shows the field induced change of the in-plane $m_{iz}^{(R)}$ and out-of-plane $m_{iz}^{(\perp)} = m_{iz}^{(R)}$ projections, $m_{iz} = \langle \hat{\Phi}_{iz}^{(R)} | \hat{S}_{iz}^{(R)} | \hat{\Phi}_{iz}^{(R)} \rangle$, $n=x,y,z$, of the individual spins $S_i$ of the ground state $\Phi_{iz}^{(R)}(S_{iz} = 1)$ in positive $B_x$ $D_z = D_x = \pm 0.5K$, $D_y = 0$, $J = 4.8K$. The spin structures of the DM model with the $D_x$ coupling differs from the only in-plane spin structures in Figs. 3, 4 of the $H_{DM}$ model by the appearance of the significant out-of-plane (Z) spin fluctuations, $m_{iz}^{(R)} = m_{iz}^{(\perp)} = -m_{iz}^{(R)} / 2$. The $m_{1x}^{(R)} = m_{2x}^{(R)}$ and $m_{3x}^{(R)}$ values of GS $I_1^{RL}(B_x)$ correspond to intermediate spin $S_{iz} = 1$ in HF $B_x$: $m_{1x}^{(R)} \to 1/6$, $m_{2x}^{(R)} = m_{3x}^{(R)} \to -1/3$, $M_{iz} \to -1/2$, $S_{iz} = 1$. The $m_{iz}^{(R)} = m_{iz}^{(\perp)}$ and $m_{iz}^{(R)}$ values of $\Pi_x^{RL}$ in Fig. 1 correspond to $S_{iz} = 0$ in HF $B_x$: $m_{iz}^{(R)} \to -1/2$, $m_{iz}^{(R)} = 0$, (Fig. 6c) $M_{iz} \to -1/2$, $M_{iz} = 0$. The spin projections change the sign in the negative field $B_x$. The pictures of the spin canting $\theta_i$ for $S_i$, $S_2$ and $S_3$ in GS $I_1^{R}$ and $I_1^{L}$ are shown schematically in the Schemes 1) for $\kappa_R > 0$ and 2) for $\kappa_L < 0$ in Fig. 6a, $tg\theta_{iz}^{RL} = m_{iz}^{(R)} / m_{iz}^{(L)}$, $k = 1,2,3$.

Figure 6b shows the KNB polarization $P_1^{R}(B_x)$ $[P_1^{L}(B_x)]$ of the $I_1^R$ $[I_1^L]$ GS and the spin canting schemes 1a) $\{2a\}$ for $B_x > 0$ and 1b) $\{2b\}$ for $B_x < 0$ at $B_{AC} \{-B_{AC}\}$ with reversing $B_x$ along the $X$-axis. Maximum $P_1^{RL}$ in Fig. 6b corresponds to the maximum out-of-plane $m_{iz}^{(R)}$ fluctuations and maximum change of the in-plane projections at $B_{AC}$ in Fig. 6a. The out-of-plane fluctuations and change of the in-plane projections of $S_i$ result in the significant out-of-plane and in-plane canting of the $S_i$, $S_2$ and $S_3$, as shown in Figs. 6 and 7. Similar field behavior of the GS $m_{iz}^{R}$ and $-m_{iz}^{L}$ of $V_3^{R}$ and $V_3^{L}$ in the vicinity of $B_{AC}$ in Fig. 6a explains the same (in magnitude) field dependence of $P_1^{R}(B_x)$ and $P_1^{L}(B_x)$ for $B_x > 3T$ in Figs. 2 and 6b, despite grate
The difference between $P^{R}(B_z)$ and $P^{L}(B_z)$ in the field $B_z$ PZ (Figs. 2, 9 [32]). The $m_{m}^{R(L)}$ spin projections and the Schemes of the $S_{i}$ ($S'_{i}$) canting in the excited $I^{L}_{x}$ ($III^{L}_{x}$) state of $V^{L}_{x}$ are shown in Fig. 6c. The spatial Scheme 1 shows the $S_{i}$ spin canting for $III_{x}^{L}$ (see Fig. 7a) opposite to that for $S_{i}$ in GS $I^{L}_{x}$ in the Scheme 2 of Fig. 6a.
Fig. 6 a) The in-plane and out-of-plane $m_{m}^{LR}$ spin projections, the schemes of the $S_1$ spin canting in transverse field $B_x$. b) The spatial schemes 1a), 1b) and 2a), 2b) of the canting of the $S_1$ spins in GS of $V_{3x}^{R}$ ($\kappa_{R} > 0$), $V_{3x}^{L}$ ($\kappa_{L} < 0$) at $B_{AC}$, $-B_{AC}$ and corresponding polarization $P_{LR}^{R/L}(B_x)$ in the KNB model and the toroidal moments $T_{y}^{R/L}(B_x)$ in transverse field $B_x \parallel X$. 1a) - $B_x > 0$; 1b) - $B_x < 0$. c) The $m_{m}^{R/L}$ spin projections and the spatial Scheme 1) [2)] of the $S_1$ spin canting in the excited $\text{III}^L$ ( $\text{II}^L$) state of $V_{3x}^{L}$, $B_x > 0$.

The out-of-plane $m_{1z}^{LR}$ and $m_{2z}^{LR} = m_{1z}^{LR}$ spin fluctuations of the opposite signs at the apices 3 and 2, $m_{3z}^{LR} = -2m_{2z}^{LR}$, in Fig. 6a, result in an appearance of the in-plane toroidal moments $T_{y}^{LR}(B_x)$ in Fig. 6b show the $D_x$-induced in-plane toroidal moment $T_{y}^{LR}(B_x)/r = \mu_B (m_{3z}^{LR} - m_{1z}^{LR})$ of GS $I_x^{R}$ ($I_x^{L}$) GS; $T_{y}^{LR}(B_x) || Y$, $T_{y}^{LR}(B_x) \bot B_x$, $T_{y}^{LR}(B_x) \bot P_{z}^{LR}(B_x)|| Z$, as shown in the Schemes 1a), 2a) for $\kappa_{R} > 0$ and 1b), 2b) for $\kappa_{L} < 0$. The in-plane $T_{y}^{LR}(B_x)$ reaches the maximal value at ALC field $B_{AC}^{y}$, where $(m_{3z}^{LR} - m_{1z}^{LR})$ possesses the maximum. The $T_{y}^{LR}(B_x)$ changes the direction in the negative field, $T_{y}(B_x) = -T_{y}(-B_x)$, Fig. 6b.

For $B_x > 0$, the LF $I_x^{R}$ ($I_x^{L}$) represents the positive (negative) chiral state with the small $D_x$ admixture of the $|3/2, M_x = -3/2>_x$ and $|3/2, M_x = 1/2>_x$. The $|3/2, M_x = 1/2>_x$ contribution to the GS is negligibly small for $B_x > 3T$ and can be neglected. In this approximation, the KNB $P_{x}^{R}(h_x)$, toroidal moment $T_{y}^{R}(h_x)$, spin chirality $\kappa_{L}^{R}(h_x)$, $\kappa_{L}^{R}(h_x)$, and the projections $M_{I_x}$, $M_{I_{II}}$ of the total $S_1$, $S_2$ spins of the $I_x^{R}$, $I_{II}^{R}$, have the following form for $B_x > 3T$

$$P_{x}^{R}(h_x) \approx 9AD_x(1 + h_x / e_x^2) / 64\Delta_x = 3\sqrt{3}\text{sign}(D_x) A m_{3z}^{I} / 4,$$

(9)
\[ T^R_r(h_x) \approx 3\sqrt{3}g\mu_B |D_x| (1 + h_x / \varepsilon_x^0) / 32 \Delta_x = 3\mu_B \mu_3 / 4, \]
\[ \kappa^R_{\parallel}(h_x) \approx \gamma (1 + \varepsilon_x / \Delta_x) \Delta_0 / \varepsilon_x^0, \quad \kappa^R_{\perp}(h_x) \approx \Delta_0 / \varepsilon_x^0, \quad \kappa_{\parallel}(h_x) = \pi / \varepsilon_x^0, \quad \chi_{\parallel}(h_x) = \pi / \varepsilon_x^0, \]
\[ M_{\parallel} = -\gamma_i(h_x / \varepsilon_x^0) (1 + \varepsilon_x / \Delta_x) + 3(1 - \varepsilon_x / \Delta_x)] = -\gamma_i[\frac{\gamma_i}{\pi} \left(1 - \kappa_{\parallel}^2 - 3(1 - \frac{\gamma_i}{\pi})\right)], \]
\[ M_{\perp} = -\gamma_i / 2 + \varepsilon_x^0 = -\gamma_i / \sqrt{1 - \kappa_{\parallel}^2}; \quad \mu_{\parallel} = 2\mu_B M_{\parallel}; \]
\[ \varepsilon_x = \sqrt{\Delta_x^2 + h_x^2}, \Delta_x = \varepsilon_x^2 + 2D_x (1 + h_x / \varepsilon_x^0) / 64)^{1/2}, \varepsilon_x = \frac{1}{4} (3J + 2\varepsilon_x^0 - 6h_x), \]

where \( \Delta_0 = \sqrt{3} / 2 \), (\( M_{\parallel} = M_{\parallel} = 0, M_{\perp} = M_{\perp} = 0 \)). Eq. (9) describes the field increase of the KNB polarization \( P_1^R(B_x) \), the maximum \( P_1^R(B_{AC}^\perp) \) at \( B_{AC} \), and subsequent decrease of \( P_1^R \) at HF in Fig. 2. \( P_1^R(B_{AC}^\perp) \) max; 3AD_x \sqrt{2} / 8 |D_x| \ in the case \( D_y = 0 \) describes the relation \( P_1^R(B_{AC}^\perp) \) max / P_1^R(B_{AC}^\perp) max = \sqrt{2} between the maximum magnitudes of the KNB \( P \) in the field \( B_z \), PZ [32] and \( B_x \perp Z \) (see Fig. 8). Both \( P_1^R(B_x) \) (9) and \( T_1^R(B_x) \) (10) are proportional to the out-of-plane \( m_{\parallel} \) spin fluctuation as shown in Figs. 6a, 6b. Equation (11) describes the field dependence of the positive chirality \( \kappa^R(B_x) \) of \( \mathbf{I}_x^L \) and its vanishing after \( B_{AC}^\perp \) in Fig. 5 and the smooth decrease of \( \kappa_{\parallel}^R(B_x) \) of \( \mathbf{II}_x^L \) without vanishing at \( B_{AC}^\perp \) (Fig. 5). The \( M_{\parallel} \) (12) \( M_{\parallel} = \sum m_{\parallel} \) changes from the ZF \( M_{\parallel} = 0 \) to \( M_{\parallel} = -1 / 2 \) and then to \( M_{\parallel} = -3 / 2 \) in accordance with Figs. 6a and 1, whereas the \( M_{\parallel} \) changes from ZF \( M_{\parallel} = 0 \) to HF \( M_{\parallel} = -1 / 2 \). Eq. (12) shows the non-linear correlation between the GS magnetic moment \( \mu_{\parallel}(B_x) = 2\mu_B m_{\parallel} [M_{\parallel}] \) and the spin chirality \( \kappa^R(B_x) \) in transverse field. The non-linear behavior of the static magnetization \( \mu \) of \( V_3 \) ring of \( V_{15} \) SMM in \( B \perp [20] \) was explained [25, 26] in the \( D_x \), \( D_y \) model.

Fig. 7a shows the change of the spin canting of the \( S_1, S_2, S_3 \) spins in GS \( \mathbf{I}_x \) (Schemes 1,2) and second ES III-III \( \mathbf{I}_x \) (Schemes 3,4) of the avoided LC structure of \( V_3 \) in transverse field \( B_x \). The field-induced \( \{ \theta_1, \zeta_1, M_1; \theta_2, \zeta_2, M_2; \theta_3, M_3 \} \) spin-canting includes the change of the out-of-plane \( \theta_1 = \theta_2 \) (for \( S_1, S_2 \)), \( \theta_3 \) (for \( S_3 \)) and in-plane \( \zeta_1 = \varphi(I) \) (for \( S_1, S_2 \)) spin canting angles, which is accompanied by the significant variations of the value of the \( M_3 \) projection of \( S_3 \) and \( M_1 \) projection on the \( XZ \) plane of the \( S_1 (S_2) \) spin of GS \( \mathbf{I}_x \) of \( V_3 \), in accordance with Fig. 6a.

The \( S_i \)-arrows in Fig. 7a schematize the directions and the magnitudes of \( S_i = \ll S_i \gg \): the lengths of arrows and the numbers among them denote the magnitudes of projections \( M_3, M_1 \) on the \( XZ \) plane and corresponding \( B_x \), respectively. Large out-of-plane spin fluctuations \( m_{i z} = m_{2 z} \) and \( m_{3 z} = -m_{1 z} \) (Fig. 7a) of the opposite signs for \( S_1, S_2 \) and \( S_3 \), respectively, and the change of the in-plane \( m_{i p} = m_{2 p} \) and \( m_{3 p} \) projections (Fig. 7a) lead to a significant out-of-plane field-dependent canting on the angles \( -\theta_1(I), (\theta_2 = \theta_2) \), and \( +\theta_3(I) \) for the \( S_1, S_2 \) and \( S_3 \) spins in GS \( \mathbf{I}_x \) in Figs. 7a and 7c, \( t g \theta_1 = m_{i z} / m_{i p}, t g \theta_2 = m_{i z} / m_{i p} \). The \( S_1, S_2 \) spins of \( \mathbf{I}_x \) rotate around the 1,2
apices (canting angle $\theta_1 = \theta_2$) up to the maximum $\theta_1 = \theta_1^\prime$; 27° at $B_{AC}$ and then rotate back that is accompanied with the change of the in-plane $\zeta = \varphi(I)$ canting angle (Figs. 7a-7c) and increase of $M_1(= M_2)$ from LF $M_1 = +0.333$ to HF $M_1 = M_2 = -1/2$.

The Scheme 4) in Fig. 7a show the simultaneous opposite dynamics of the $S_i^0(S_2^0)$ spins in the ES III, with the accompanied decrease of $M_1 = M_2 = -1/2$ [ $S_{ex} = 3/2$ ] to HF $M_1 = M_2 = -1/3$ [ $S_{ex} = 1/2$ ]. The $M_j^i(B_x)$ projection of $S_j$ in III (Scheme 3) exhibits the clockwise non-linear $\xi_3$-rotation in the XZ plane around the vertex 3 at almost $\xi_3 \approx 180^\circ$, which is opposite to the $\theta_3$-rotation of $M_j$ in the Scheme 1 for $I^L_x$, $\eta_3(B_{AC}^x) = \pi - \xi_3(B_{AC}^x) = \theta_3(B_{AC}^x)$ [Figs. 7a, 7c]. This $M_j(B_x)$ rotation is accompanied with the reduction of $M_3$ from the ZF $M_{3z} = -1/2$ [ $S_{ex} = 3/2$ ] to the HF $M_{3z} = +1/6$ [ $S_{ex} = 1/2, S_{12} = 1$ ]; $M_j(B_{AC}^x) = M_j(B_{AC}^x)$. The field

![Fig. 7a](image-url)
Fig. 7. Field-induced $[\theta_1, M_\perp]$ spin canting in $V_{3x}^L$ with the $D_\perp$ coupling in transverse field $B_x$.

a) The schemes of the field-induced out-of-plane spin canting and an accompanying increase of the $M_3$ (the Scheme 1) and the $M_{1\mid XZ}$ projection (2, $B_x > 0$, and 4, $B_x < 0$). $B_x > 0$; a) The schemes of the field-induced out-of-plane $\theta_1$ and $\theta_I$ spin canting and an accompanying increase of the $M_3$ (the Scheme 1) and the $M_{1\mid XZ}$ projection (2, $B_x > 0$, and 4, $B_x < 0$). $B_x > 0$; b) The correlations between the vector chirality $R(L)_{ix}$, the in-plane $m_{ix}$ spin fluctuations and $\zeta$-canting of the $S_I$, $S_2$ and polarization $P_{1R(L)}^{RI}(B_x)$. c) The field ($B_x$) dependence of the angles of the out-of-plane $\theta_1(I)$, $\theta_I(I)$, $\xi_{3}(III)$, $\xi_3(III)$, $\eta_3(III)$ and in-plane $\zeta$ ($= \varphi_1(I)$), $\varphi_{II}$, $\varphi_{III}$ spin canting for the $\Pi^L_{x}$, $\Pi^L_{II}$, $\Pi^L_{III}$ states. d) The schemes of the spin canting, polarization, toroidal moments and spin chirality of the GS $\Pi^L_{x}$ and $\Pi^L_{II}$, $\Pi^L_{III}$ ES of the avoided LC structure in transverse field $B_x$. The spin structures 1), 2) and 3) are shown for the bottom (at $\Pi^L_{x}$), center ($\Pi^L_{II}$), and top ($\Pi^L_{III}$) of the tunneling gap $\Delta_{tx}$ at ALC field $B_{AC}^\perp$.
induced spin dynamics for the $M_1, M_2$, and $M_3$ is in accordance with the $[S_{\chi} = 3/2 \rightarrow S_{\chi} = 1/2]$ spin transition in the III$_x$ of the avoided LC structure in transverse field $B_x$.

Fig. 7b shows the change of the in-plane spin $\zeta$-canting of the in-plane $m_{1p}$, $m_{2p}$ projections ($|m_{1p}| = |m_{2p}|$) of the $S_1, S_2$ vectors and the spin chirality $\kappa^R(x)(B_x)$ of the GS $I^R, I^L_x$ of $V^R_{3x}, V^L_{3x}$ with the $D_x$ coupling in the field $B_x$. The spin structures in Figs. 7a and 7b differ significantly from the spin schemes in Figs. 3b and 4a in the $H^I_{DM}$ model with $m_{1z} = 0$ due to the large $m_{1z} = m_{2z}$ and $m_{3z} = -2m_{1z}$ out-of-plane spin fluctuations in GS with the maximum $Z$-projections at $B^C_{AC}$, Figs. 6a and 7a. In transverse field $B_x \perp Z$, the field-dependent vector spin chirality $\kappa_1(B_x) [\kappa_1(B_x) \parallel Z]$ is not only the quantum characteristics of GS $I^R, I^L_x$, but also has a direct physical meaning: $\kappa_1(B_x)$ describes the in-plane spin fluctuations $m_{1y} (m_{2y})$ and the $\zeta(B_x)$-canting (rotation) of the $S_1, S_2$ and can be directly accessed by the measurements of the in-plane canting angle $\zeta(B_x)$ of $S_1, S_2$ in the increasing field $B_x$ (Fig. 7b) in the NMR and polarized NS experiments on the single crystal $V_3$ system.

Fig. 7c shows the field ($B_x$) dependence of the simultaneous change of the angles of the out-of-plane $\theta_1(I), \theta_2(I), \phi_1, \phi_2$, $\phi_1$ canting for $S_1$ ($S_2$) and $S_3$ for the $I^L_x, II^L_x, III_x$ states of $V^L_{3x}$ ($\kappa^L_{1} < 0$). Figs. 6a, 7a-7c describe the $[\theta, \phi, \eta, \zeta, \phi_1, M_1]$ spin-canting of the individual $S_i$ spins in the field $B_x$. The dynamics of the spins in GS $I^R, I^L_x$ in the transverse field $B_x \perp Z$ significantly differs from that in the field $B_z PZ$[31, 32].
Fig. 7d shows the three-level avoided LC structure in the vicinity of the \( \Delta \) tunneling gap at the ALC field \( B_{AC}^x \) of \( V_{3x}^l \): the ground \( I_x^l \) state \([ \Phi_{ir}(S_{12} = 1) ]\) which describes the \([ |S_x^1 = 1/2 >_x, |S_x^2 = 3/2 >_x] \) transition from the spin-frustrated to the spin-collinear state in \( B_x^l \), first excited \( \Pi_x^l \) \([ \Phi_{ir}(S_{12} = 0) ]\) linear level and the second excited \( \Pi_x^l \) \([ \Phi_{ir} ]\) state, which describes the \([ |S_x = 3/2 >_x, |S_x = 1/2 >_x] \) spin transition. Fig. 7d also shows the \( S_1, S_2, S_3 \) spin-canting schemes 1) and 3) in the bottom \((I_x^l)\) and top \((\Pi_x^l)\) of the tunneling gap \( \Delta \) at \( B_{AC}^x \), respectively, as well as the spin scheme 2) of the ES \( \Pi_x^l \) at the center of \( \Delta \). The maximum GS KNB \( P_{ir}^l(B_x^l) \) and the in-plane \( T_{iy}^l(B_x^l) \) at \( B_{AC}^x \) are shown by the vertical \((|| Z)\) and horizontal \((|| Y)\) solid arrows, respectively. The \( S_1, S_2, S_3 \) canting scheme 3) for the \( \Pi_x^l \) state on the top of the gap \( \Delta \) is opposite to that in the Scheme 1) of \( I_x^l \), that results in the opposite sign of the maximum \( P_{ir}^l(B_x^l) \) and \( T_{iy}^l(B_x^l) \) of \( \Pi_x^l \) in comparison with \( P_{ir}^l(B_x^l) \) and \( T_{iy}^l(B_x^l) \) of GS. The opposite spin structures in the Schemes 1) and 3) in Fig. 7d explains different signs of the \( P_{ir}^l(B_x^l) \) and \( P_{ir}^l(B_x^l) \) in Fig. 2. All three spatial spin Schemes of the states \( I_x^l, \Pi_x^l, \Pi_x^l \) of the gap \( \Delta \) at \( B_{AC}^x \) in Fig. 7d are characterized by the intermediate spins \( S_{12} \), small vector chirality and zero scalar chirality \( \chi_N(B_x^l) = 0 \). The spin Scheme 2) of the first ES \( \Pi_x^l \), which corresponds to \( S_{12} \rightarrow 0 \) (see also \( \Pi_x^l \) in Fig.3b), and \( \kappa_{ir}^l(B_{AC}^x) = -0.12 \), very small out-of plane spin canting due to very weak ZF DM(x) admixture that leads to the small \( P_{ir}^l(B_x^l) \) (Figs. 2) and \( T_{iy}^l(B_x^l) \). The spin chirality \( \kappa_{ir}^l(B_x^l) \) of the spin-frustrated GS \( I_x^l \) \((S_{12} = 1)\), which tends to zero at HF \( B_x^l > B_{AC}^x \), is transferred by the \( D_x \) coupling in increasing field to the to the \( \Pi_x^l \) state \((S_{12} = 1)\), which was spin-collinear \((S = 3/2, \kappa = 0)\) initially, that results in \( \kappa_{ir}^l(B_{AC}^x) = \kappa_{ir}^l(B_{AC}^x) = -0.06 \) at \( B_{AC}^x \), \( \kappa_{ir}^l + \kappa_{ir}^l = \kappa_{ir}^l \). The in-plane and out-of plane dynamics of the spin canting in the states of the avoided LC structure of \( V_{3x}^l \) in transverse field \( B_x \perp Z \) (Fig. 7) differ significantly from that in the field \( B_z PZ \) [31, 32].

Figure 8 shows the comparison of the field dependence of the KNB polarization \( P_{z}^{R(l)}(B_z) \) and \( P_{z}^{R(l)}(B_z) \) of \( V_{3x}^l \) in a single-crystal sample at temperature \( T = 0.1 K \), when essentially only the GS is temperature populated, \( B_z > 0 \). In the field \( B_z PZ \), the polarization \( P_{z}^{l}(B_z) \) (open triangles) is close to zero up to LC field, \( |B_z| > |B_{A1}^x| \), for \( V_{3x}^l \) with GS \( I_x^l \) \((\kappa_l^l = -1)\) [32]. The maximum \( P_{z}^{max}(B_{A1}^x) \) of the \( P_{z}^{l}(B_z) \) of \( V_{3x}^l \) at the ALC \( B_z \)-field \( B_{A1}^x \) smaller in magnitude than the maximum \( P_{z}^{max}(B_{A1}^x) \) of the \( P_{z}^{l}(B_z) \) polarization of \( V_{3x}^l \) with GS \( I_x^l \) \((\kappa_l^l = 1)\). The maximum of the polarization \( P_{z}^{l}(B_z) \) at transverse "resonance" field \( B_{AC}^x \), \( P_{z}^{max}(B_{AC}^x) \), is larger in value than the maximum \( P_{z}^{max}(B_{A1}^x) \) at \( B_{A1}^x (B_z PZ) \) for \( V_{3x}^l \). At the same time, the maximum polarization \( P_{z}^{max}(B_{AC}^x) \) at \( B_{AC}^x (B_z \parallel X) \) is smaller than the maximum polarization
The rotation of the fixed applied field \(B_{z1} = B_{A1}^{\prime}\) in the \(ZX\)-plane \((B_{z1} P Z \rightarrow B_{1x} \parallel X, \ |B_{1x}| = |B_{z1}|)\), results in the reduction \(\Delta P^{R}_{z}(B_{z2} \rightarrow B_{1x})\) \([-46\%\ of\ P_{max}^{L}(B_{A1}^{\prime})]\) of the polarization. For \(V^{L}_{3x}\), the polarization \(P_{max}^{L}(B_{z1})\) does not change practically the value under this rotation. The rotation \(B_{2z} \parallel X \rightarrow B_{2z}, P Z\) of the direction of the fixed transverse "resonant" field \(B_{2x} = B_{AC}^{x}\) for the \(P^{L}_{z}(B_{x})\) results in a significant decrease \(\Delta P^{R}_{z}(B_{2x} \rightarrow B_{2z})(-80\%\ of\ P_{max}^{L}(B_{2x}))\) of the magnitude of \(P_{z}^{L}\) of \(V^{L}_{3x}\) while the same rotation leads to \(-40\%\) increase \(\Delta P^{R}_{z}(B_{2x} \rightarrow B_{2z})\) of \(P_{z}^{R}\) of \(V^{R}_{3x}\).

Toroidal moments \(T\) in Fig. 8 change the value from the maximal \(T_{y}^{R(L)}(B_{2x})|_{max}\) \(Y\) value at the transverse ALC field \(B_{2x} = B_{AC}^{x}\) to zero value \(T(B_{z}) = 0\) under the field rotation \(B_{z1} \parallel X \rightarrow B_{z2}, P Z\). The field dependence of the polarization \(P^{R(L)}\) in the KNB model and the toroidal moments \(T^{R(L)}\) show strong anisotropy: \(P^{R(L)}\) and \(T^{R(L)}\) differ significantly in the fields \(B \parallel Z\) and \(B \perp Z\).

In transverse field \(B_{y}, P Y\), the \(V^{R}_{3x}, V^{L}_{3x}\) systems \([D_{z} = D_{x} = m0.5K, D_{y} = 0, J = 4.8K]\) possess the \(m_{m}(B_{y})\) field dependence and the in-plane spin structures, which correspond to GS with \(S_{12} = 0\) (Schemes \(Ia - Ie\) \([Ia^{\prime} - Ie^{\prime}]\) in Fig. 9a) mixed with the \(\{3/2,M = -3/2\}_y\) by the \(D_{x}\) DM coupling. Figure 9a \((B_{y} \geq 0)\) shows the
transformations of the in-plane spin structures, total spin projections $M_y = M_y^I, M_y = M_y^R$, individual in-plane $m_{ip}$ spin projections, canting angles $\phi$ and spin chirality of $V_{3s}^R (V_{3s}^L)$ systems $I, II (I', II')$ with positive (negative) spin chirality of the GS $I (I')$ with $S_{12} = 0$, and first ES $II (II')$ with $S_{12} = 1$.

Fig. 9b shows the in-plane $m_{ix}, m_{iy}, m_{ip} = m_{2p}$, the out-of-plane $m_{iz}, m_{2z}$, and total $|M_1| = |M_2|, M_3$ spin projections, polarization $P_{z}^B (B_y)$, toroidal moment $T_n^+ (B_y)$, the Schemes 1-3 of the out-of-plane (1, 2) and in-plane (3) spin canting, and the change of the in-plane $\phi$ and out-of-plane $\eta$ spin canting angles for GS of $V_{3s}^L$. The out-of-plane spin fluctuations $m_{iz}$ (solid curve) and $m_{2z} = -m_{iz}$ (dash) of the opposite signs reach the maximum at $B_{AC}^\ast$, $m_{3z} = 0$. The $m_{iy} = m_{2y}$ projections (short-dash-dot) change the value from the low-field $m_{iy} = +1/6$ to the high-field $m_{iy} = -1/2$, that corresponds to the rotations of the $S_1, S_2$ spins in the $YZ$ plane (Scheme 2) around the 1,2 apices at the angle $\eta \approx 2\pi$ accompanied by the in-plane $\phi$-canting and the change of the $|M_1| = |M_2| (solid)$ and $M_3$ projections. The Scheme 2 shows this rotation of the $M_1 |_{YZ}$ projection on the $YZ$ plane (dotted curve in Fig. 9b). The lengths of the arrows and the numbers among them in the Scheme 2 show the values of $M_1(B_y) |_{YZ}$ and the corresponding $B_y$ values, respectively. At HF ($B_y > 5 T$), the $M_1(B_y) |_{YZ}$ value coincides with the total $|M_1|$ projection of $S_1$ in Fig. 9b. The change of the opposite $m_{iz}$ and $m_{2z}$ out-of-plane spin fluctuations, shown by the dash-dotted vertical arrows at the apices 1 and 2 in the spatial Scheme 1 in the vicinity of LC field $B_{AC}^\ast$, results in
Fig. 9b

The in-plane toroidal moment $T_{tx}(B_y) = \frac{1}{2} g \mu_B \left( [r_1 \times S_1] + [r_2 \times S_2] \right) = \frac{1}{2} g \mu_B r m_{ix}$, $T_{tx}(B_y) \perp B_y$, $T_{tx}(B_y) \perp P_{ix}(B_y)$. $T_{tx}(B_y)$ reaches the maximum at $B_{AC}$ since $T_{tx}(B_y) - m_{ix}$. This $T_{tx}(B_y)$ corresponds to significantly different spatial spin structure (Scheme 1 in Fig. 9b) in comparison with that for the field $B_x \parallel X$ (Figs. 6 and 7), however the $T_{tx}(B_y)$ curve coincides with the $T_{tx}(B_y)$ curve in Fig. 6b, $T_{tx}(B_y) = T_{tx}(B_y)$ $T_{tx}(B_y) = \frac{1}{2} g \mu_B \left( [r_1 \times S_1] + [r_2 \times S_2] + [r_3 \times S_3] \right) = \frac{1}{2} g \mu_B r (m_{ix} - m_{iz})$. The field dependence $P_{ix}(B_y)$ in $B_x \parallel Y$ with the maximum at $B_{AC}^y$ ($B_{AC}^y = B_{AC}^z$) coincides with $P_{ix}(B_x)$. $P_{ix}(B_x)$ is isotropic in the $XY$-plane. The toroidal moment of $V_{3x}^R$, $V_{3x}^L$ with $D_y = 0$ is equal to zero in the field $B_x \parallel Z$, Fig. 8.

7. Toroidal moment induced by the $D_y$ spin mixing in transverse field

The spin structure, spin canting, chirality and polarization strongly depends on the $D_x$, $D_y$, $D_z$ and $J$ exchange parameters and the direction of the magnetic field $B$. It was shown [333] that $V_{3y}^R$ with the $D_y$ coupling [$J = 4.8 K$, $D_z = D_y = -0.5 K$, $D_x = 0$] in magnetic field $B_x \parallel Z$ possesses toroidal moment

$$T_z = \frac{1}{2} \mu_B g \sum_i [r_i \times S_i]. \quad (13)$$
The toroidal moment $T_x(B_z)$, induced by the $D_y$ spin-mixing, increases in an increasing field $B_z$, reaches the maximum at the ALC field $B_{A1}$, and then gradually decreases, $T_x(B_z)$ changes the direction in the negative field, $T_x(B_z) = -T_x(-B_z)$ [31, 32]. Fig. 10a shows the field dependence of the in plane $m_{iz}$ projections, the out-of-plane $m_{iz}$ spin fluctuations, the scheme of the spin canting in the $(S_1, S_2, S_3)$ system and the toroidal moment $T_{ix}(B_x)$ for $V_{3x}$ in transverse field $B_x \parallel X$. The $D_y$ coupling results in the large out-of-plane $m_{iz}$ and $m_{2z} = -m_{iz}$ spin fluctuations of $S_1, S_2$ in the vicinity of $B_{AC}^x$, which are oriented in opposite directions, as shown in the Scheme 1) in Fig. 10a for $B_x > 0$. The out-of-plane spin fluctuations $m_{iz}, m_{2z}$ reach the maximum magnitude at $B_{AC}^x$ that leads to the large out-of-plane canting angle $\xi_1 (\xi_2)$ and small in-plane canting $\zeta_1 (\zeta_2)$ for the spin $S_1 (S_2)$ at $B_{AC}^x$ in the Scheme 1 in Fig. 10a [\(\xi_1 = -54^\circ, \xi_2 = 54^\circ, \zeta_1 = 3^\circ, \zeta_2 = -3^\circ\)]. The $S_3$ with the variable $M_z = m_{3z}$ length is directed along the X-axis, $m_{3x} = m_{3y} = 0$. These opposite directions of the $S_1, S_2$ fluctuations along the Z-axis lead to the anticlockwise twisting spin moment around the X-axis in the ZY plane that, in turn, results in the toroidal moment $T_{ix}(B_x) = \sqrt{3} \mu_B r_0 m_{iz}$, oriented in the plane of the triangle along the X-axis in the Scheme 1 in Fig. 10a. The in-plane toroidal moment $T_{ix}(B_x)$ reaches the maximum magnitude at $B_{AC}^x$ in Fig. 10a. The Schemes 1 ($B_x > 0$) and 2 ($B_x < 0$) of the spin canting in Fig. 10a and the $T_{ix}(B_x)$ curve show that the toroidal moment $T_{ix}(B_x) \parallel X$ changes the direction upon the field $B_x$ reversal. $T_{ix}(B_x) = -T_{ix}(-B_x)$.

In Fig. 10b, the toroidal moments $T_z^{RL}(B_x), T_x^{RL}(B_x)$ and the vector spin chirality $\kappa_z^{RL}(B_x), \kappa_x^{RL}(B_x)$ of $V_{3x}$, $V_{3x}^L$ in the field $B_x \parallel Z$ and $B_x \parallel X$ at temperature $T = 0.1K$ are compared. The decrease of the positive vector chirality $\kappa_z^{RL}(B_x)$ of $V_{3x}^R$ in the increasing $B_x$ is accompanied by an increase of $T_x(B_x)$, the maximum $T_x(B_{AC})$ at $B_{AC}^x$ corresponds to the maximum of $d\kappa_z/\theta B_x$ at $B_{AC}^x$. In an increasing filed $B_x$, the toroidal moment $T_z^R(B_x) \parallel Z$ of $V_{3x}^R$ reaches the maximum magnitude $T_z^R(B_{AC}^x)$ at $B_{iz} = B_{A1}$. The subsequent rotation $B_x \parallel Z \rightarrow B_x \parallel X$ of the fixed $B = B_{iz}$ in the ZX plane results in the rotation and reduction of the toroidal moment $T$ since in Fig. 10b. In increasing $B_x$, the toroidal moment $T_x^{RL}(B_x)$ reaches the maximum $T_x^{RL}(B_{AC}^x)_{\text{max}}$ at $B_{iz} = B_{A1}^x$. Fig. 10b. The subsequent rotation $B_x \parallel X \rightarrow B_x \parallel Z$ of the fixed field $B = B_{ix}$ in the XZ plane results in the rotation of $T_x^{RL}(B_x) \parallel X \rightarrow T_x^{RL}(B_x) \parallel Z$ of $T$ and an increase (decrease) of $T^R (T^L T^+)$. The left chirality $\kappa_z^{L}(B_x)$ of $V_{3x}^L$ changes the sign at LC field $B_{iz}$, the right chirality $\kappa_z^{R}(B_x)$ of $V_{3x}^R$ demonstrates significant field dependence, Fig. 10b. Different vector spin chirality $\kappa_z^{L}(B_x)$ and $\kappa_z^{R}(B_x)$ of $V_{3x}^L, V_{3x}^R$ in the field $B_x$ transform into $\kappa_z^{R}(B_x)$ and $\kappa_z^{L}(B_x)$ in transverse $B_x$, respectively, which have the same form and differ by the sign.
Fig. 10 a) Field dependence of the $m_{in}$ spin projections, spatial schemes of the spin canting and toroidal moments $T_{ix}(B_x)$ for $V_{3z}$ in transverse field $B_x \parallel X$, 1) $B_x > 0$, 2) $B_x < 0$. b) Toroidal moments $T_{ix}^{R(L)}(B_x)$, $T_{ix}^{R(L)}(B_x)$ and the vector chirality $\kappa_{z}^{R(L)}(B_x)$, $\kappa_{x}^{R(L)}(B_x)$ of $V_{3x}$, $V_{3x}$ in the field $B_z \parallel Z$ and $B_x \parallel X$ at temperature $T = 0.1K$.

8. Conclusion
The inverse DM mechanism of polarization $\mathbf{P}$ [39-41] is the driving force of the polarization $P_z(B_x)$ induced by the $D_x$ coupling in transverse magnetic field $B_x$ in the spin-frustrated $V_3$ SMM with the out-of-plane and in-plane DM interaction. The $D_x$ induced KNB polarization $P_z(B_x)$ increases non-linearly with increasing field $B_x$, reaches a maximum at the avoided LC field $B_{AC}$ and then gradually decreases in high fields. The $D_x$ coupling in $V_{3x}$ results also in the field-induced in-plane toroidal moment $T_y(B_x) \parallel Y$ in transverse $B_x$. The origin of $P_z(B_x)$ and $T_y(B_x)$ is the large out-of-plane spin fluctuations induced by the $D_x$ coupling. The correlations between the polarization, toroidal and magnetic moments, spin chirality and spin canting in transverse field were investigated in detail. The dynamics of the individual $S_1, S_2, S_3$ spins in the ground and excited states of the avoided level crossing structure in transverse field $B_x (B_x, B_y)$ significantly differs from the spin dynamics in the field $B_x \parallel Z$. The field-induced spin canting in $B_x$ includes large canting of the $(S_1, S_2)$ and $S_3$ spins in opposite directions which is accompanied by the significant different change of the $M_i$ projections. The coupling between the vector chirality $\kappa$ and transverse field $B_x$ is non-linear. The scalar chirality is equal to zero in transverse field, $\chi(B_x) = 0$, in spite of the large out-of-plane spin fluctuations of the opposite signs and large spatial spin canting. The vector chirality $\kappa_z(B_x) \{ \kappa_y(B_y) \}$ describes the in-plane canting (rotations) of the $S_1, S_2$ spins in transverse field $B_x [B_y]$. The $D_y$ coupling in $V_{3y}$ results in the field-dependent in-plane toroidal magnetic moment $T_y(B_x) \parallel X$ in $B_x$. Under the $B_z \rightarrow B_x$ rotation of the field $B$ in the XZ plane, the polarization $\mathbf{P}$ demonstrates the reduction of the magnitude in the $P_z(B_x) \rightarrow P_y(B_y)$ transition, while the toroidal moment $T_y$ exhibits the $T_z(B_y) \rightarrow T_x(B_x)$ flop. The DM $V_3$ nanomagnets are the cluster analogs of multiferroics.

**Appendix A**

In the spin chirality representation, the wave functions of the zero-field double degenerate GS (I, II) of the $V_3$ trimer in the $H_{DM}^i$ model $(D_p = 0)$ with $D_z < 0$ in transverse field $B_x$ has the form

$$\Phi_{l_k} \{ \Phi_{l_k} \} (D_z < 0) = n_1 \Omega^L_m + [-] n_2 \Omega^R_m,$$  \hspace{1cm} \text{(A1)}

of the mixture of the states $\Omega^L_m = \Omega_m(\kappa_z = -1)$ and $\Omega^R_m = \Omega_m(\kappa_z = 1)$ with positive (right) $\kappa_z = 1$ and negative (left) $\kappa_z = -1$ chirality, respectively, where

$$\Omega_m(\kappa_z = 1) = [u_+ (-1/2) \pm u_+ (1/2)]/\sqrt{2}, \quad \Omega_m(\kappa_z = -1) = [u_+ (-1/2) \pm u_+ (1/2)]/\sqrt{2},$$

$$n_{l_{(2)}} = \frac{1}{2} \sqrt{d_z \pm \sqrt{d_z^2 + h_z^2}}.$$  \hspace{1cm} \text{(A2)}
The eigenfunctions \( u_1 = u_-(M_S = -1/2) \), \( u_2 = u_+(1/2) \), \( u_{11} = u_-(1/2) \), \( u_{12} = u_+(1/2) \), which diagonalize the \( H_{DM}(z) \) (\( D_p = 0 \)) model and eigenvalues \( E_n[u_+(M_S)] \) are presented in Eqs (A3) and (A4), respectively.

\[
\begin{align*}
\phi_0(-1/2) &= n[|z\rangle - n|\bar{z}\rangle] / \sqrt{2}, \\
\phi_0(1/2) &= n[|z\rangle + n|\bar{z}\rangle] / \sqrt{2}; \\
\phi_0(-1/2) &= n[|z\rangle - n|\bar{z}\rangle] / \sqrt{2}, \\
\phi_0(1/2) &= n[|z\rangle + n|\bar{z}\rangle] / \sqrt{2};
\end{align*}
\]  
\[
\begin{align*}
\phi_0(-1/2) &= (|z\rangle - n|\bar{z}\rangle) / \sqrt{2}, \\
\phi_0(1/2) &= (|z\rangle + n|\bar{z}\rangle) / \sqrt{2};
\end{align*}
\]  
\[
E_n[u_+(1/2)] = D_+ \sqrt{3}/2, \quad E_n[u_+(m1/2)] = -D_+ \sqrt{3}/2,
\]  
where \( \omega_+ = \exp(± 2\pi i / 3) \), \( \phi_0(M) = \phi_{S_{12}=0}(M) \), \( \phi_1(M) = \phi_{S_{12}=1}(M) \) are the spin functions characterized by the \( S_{12} \) intermediate spin, \( S_{12} = 0, 1 \).

\( V_3 \) trimer in the DM(\( z \)) model with \( D_0 > 0 \) possesses the following wavefunctions of the double degenerate GS (I, II):

\[
\Phi_{1+0}(\Phi_{0+1}) [D_0 > 0] = n_{1} \Omega_{m}(-1) \pm n_{2} \Omega_{m}(1).
\]  
(A5)

In the intermediate spin \( S_{12} \), the wavefunctions of the ZF double degenerate GS (I, II) in transverse positive field \( B_x \) in Fig. 4b

\[
\begin{align*}
\Phi_{1+}(S_{12} = 1) &= C_1 \Lambda_+(S_{12} = 1) + iC_2 \Lambda_+(S_{12} = 0), \\
\Phi_{1-}(S_{12} = 0) &= C_1 \Lambda_-(S_{12} = 1) - iC_2 \Lambda_-(S_{12} = 0)
\end{align*}
\]  
(A6)

represent the mixture of the states with \( S_{12} = 1 \) (I) and \( S_{12} = 0 \) (II) with corresponding spin structures, where

\[
\Lambda_+(S_{12}) = [\phi_{S_{12}}(-1/2) \pm \phi_{S_{12}}(1/2)] / \sqrt{2}, \quad C_{1/2} = \sqrt{\left(1 \pm \Omega \right) / \sqrt{d_x^2 + h_x^2}}.
\]  
(A7)

The field-induced transformations of the planar spin structures in Figs. 3a, 3b, 4a are determined by the dependence of the in-plane \( m_{in}^{\pm} \) projections of the \( \Phi_{ik}^0 \) and \( \Phi_{ik}^0 \) states (\( D_z < 0 \)) in the \( H_{DM}^0 \) model on \( B_x \)

\[
\begin{align*}
m_{in}^z &= m_{2z}^z = \pm \frac{1}{\sqrt{0}} \left[1 \mp h_x / \epsilon_x^0 \right], \quad m_{3z}^z = \pm \frac{1}{\sqrt{0}} \left[2 \mp h_x / \epsilon_x^0 \right]; \\
\epsilon_x^0 &= \sqrt{\Delta_0^2 + h_x^2}.
\end{align*}
\]  
(A8)

where \( B_x > 0 \), the superscripts \( \pm \) and \( \mp \) in \( m_{in}^z \) projections in Eq. (5) corresponds to the \( I \) (\( S_{12} = 1 \)) and \( II \) (\( S_{12} = 0 \)) states, respectively, \( \epsilon_x^0 = \sqrt{\Delta_0^2 + h_x^2} \). For the double-degenerate \( I' (\Phi_{ik}^0) \) and \( II' (\Phi_{ik}^0) \) states of the system with \( D_z > 0 \), the in-plane \( m_{1x}^z = m_{2x}^z \) and \( m_{3x}^z \) projections coincide with that of Eq (5), whereas the \( m_{1y}^z = -m_{2y}^z \) projections have opposite signs in comparison with that in Eq (5), that results in the in-plane spin structures \( I_x, I_y, I_c (S_{12} = 1) \) and \( II_x, II_y, II_c (S_{12} = 0) \) for \( D_z > 0 \), \( B_x > 0 \) in Fig. 3b. The values of the total in-plane spin projections \( |m_{1p}^z| = |m_{2p}^z| \) are the same for \( D_z > 0 \) and \( D_z < 0 \).

In transverse magnetic field \( B_x \), the low field ground state for \( D_z < 0 \) (\( D_z > 0 \)) represents the positive (negative) chiral state \( \Omega_+ (\kappa_x = +1) \) (\( \Omega_- (\kappa_x = -1) \)) with the small DM admixture of \( \Phi_{ik} = [\Phi_{ik}(-3/2) + \sqrt{3} \Phi_{ik}(1/2)] / 2 \) (\( \Phi_{ik} = [\Phi_{ik}(1/2) - \sqrt{3} \Phi_{ik}(-3/2)] / 2 \).
\begin{align*}
\{[\Phi(-3/2) - \Phi(3/2)] - \sqrt{3}[\Phi(-1/2) - \Phi(1/2)]/2\sqrt{2}; \quad \Phi_x(1/2) = \{\sqrt{3}[\Phi(-3/2) - \Phi(3/2)] + [\Phi(-1/2) - \Phi(1/2)]/2\sqrt{2}\} \text{ diagonalize the Zeeman interaction in transverse field [25, 30]. Thus, the GS wave functions at B=0.02T are } \Phi_{lx}^{(0.02 T)} \approx 0.9987\Omega_x(1) + i0.05\Phi_{lx} \\
\text{ for } D_x < 0 \text{ and } \Phi_{lx}^{(0.02 T)} \approx 0.9994\Omega_x(1) + i0.028\Phi_{lx} \text{ for } D_x > 0.
\end{align*}

In the vicinity of the LC point, \(B_x > 3-4T\), the DM contribution of the \(1/2\) state to the ground state \(\Phi_{lx}^{(S_{1z}=1)} \sim [\varphi_1(-1/2) - \varphi_1(1/2)]/\sqrt{2}\) is negligibly small (due to the large interstate interval \(\Delta^\prime; \ 3J/2 + g\mu_B B_x\) in Fig. 1) and can be neglected. In this case, the individual in-plane and out-of-plane projections \(m_{1n}\) of the individual spins of the \(V_3\) trimer in the ground state \(I\) can be approximated by Eq. (A12)

\begin{align*}
m_{1x}^1 &= m_{2x}^1; \quad -[(h_x/\varepsilon_x^0)(1+\varepsilon_x/\Delta_x) + 2(2-\varepsilon_x/\Delta_x)]/12, \\
m_{1x}^3 &= [5\varepsilon_x/\Delta_x - 1 - (h_x/\varepsilon_x^0)(1+\varepsilon_x/\Delta_x)]/12, \\
m_{1y}^1 &= -m_{1y}^1; \quad D_x(1+\varepsilon_x/\Delta_x)/4\varepsilon_x^0, \quad m_{3y} = 0, \quad M_{by} = M_{by} = 0; \\
m_{1z}^1 &= m_{2z}^1; \quad -\sqrt{3}|D_x|(1+h_x/\varepsilon_x^0)/32\Delta_x, \quad m_{3z} = -2m_{1z}^1; \quad M_{iz} = M_{iz} = 0,
\end{align*}

where \(\varepsilon_x^0 = \sqrt{\Delta_0^2 + h_x^2}, \quad \Delta_x = \sqrt{\varepsilon_x^2 + \nu_x^2}, \quad \varepsilon_x = \frac{1}{4}(3J + 2\varepsilon_x^0 - 6h_x), \quad \nu_x = \frac{1}{4}D_x\sqrt{1+h_x/\varepsilon_x^0}, \quad \Delta_0 = |D_x|\sqrt{3}/2\). The out-of-plane \(Z\)-projections \(m_{1z} = m_{2z}\) and \(m_{3z} = -2m_{1z}\) have opposite directions. The canting of the spins \(S_1, S_2 \) and \(S_3\) is determined by the equation

\[t_\theta \theta_1 = t_\theta \theta_2 = m_{1z} / m_{1p}, \quad t_\theta \theta_3 = m_{3z} / m_{3s}, \quad m_{1p} = \sqrt{m_{1z}^2 + m_{1y}^2}.\]

**References**

44. S.-W.Cheong, and M. Mostovoy, Nat. Mater. 6, 13 (2007).