

Magnetic structure of the kagome metal YbFe_6Ge_6 in view of Bragg diffraction

S. W. Lovesey *ISIS Facility, STFC, Didcot, Oxfordshire OX11 0QX, United Kingdom;**Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom;**and Department of Physics, Oxford University, Oxford OX1 3PU, United Kingdom*

(Received 8 June 2025; revised 10 August 2025; accepted 16 September 2025; published 1 October 2025)

A material in possession of localized $4f$ -electron magnetism and delocalized $3d$ -electron or band magnetism can often present enigmatic physical phenomena, and there has been a longstanding interest in the kagome metal YbFe_6Ge_6 . More recently, because of an investigation of a so-called anomalous Hall effect, or topological Hall effect, and magnetic neutron Bragg diffraction [Yao *et al.*, *Phys. Rev. Lett.* **134**, 186501 (2025)]. Iron moments in the two-dimensional layers of a hexagonal nuclear structure undergo collinear antiferromagnetic order below a temperature ≈ 500 K. The moments depart from the c axis in a spontaneous transition at ≈ 63 K to an orthorhombic structure. The magnetism of Yb ions appears to behave independently, which can be confirmed using resonant x-ray Bragg diffraction enhanced by a Fe atomic resonance. The inferred magnetic structure is P(parity)T(time)-symmetric (anti-inversion $\bar{1}$) collinear antiferromagnetism that does not couple to circular polarization (helicity) in primary x-rays, unlike altermagnetism. A linear magnetoelectric effect is allowed, and Kerr rotation and the piezomagnetic effect are forbidden. Symmetry informed Bragg diffraction patterns for future x-ray and neutron experiments are shown to be rich in Fe magnetic properties of orthorhombic YbFe_6Ge_6 , including space-spin correlations, anapoles, and Dirac quadrupoles familiar in high- T_c ceramic superconductors.

DOI: [10.1103/rn9y-6spg](https://doi.org/10.1103/rn9y-6spg)

I. INTRODUCTION

Ternary intermetallics RFe_6Ge_6 crystallize in closely related structures that result from insertion of the R element within the Ge_8 holes of the hexagonal host (P6/mmm) [1–3]. The magnetic properties are characterized by an antiferromagnetic ordering of the Fe sublattice above room temperature, and a stacking sequence $+ - + -$ along the hexagonal c_h axis depicted in Fig. 1. Iron moments align with this axis, and moment values range between $1.5 \mu_B$ and $2.2 \mu_B$. There is zero molecular field on the R sites, and a concomitant low ordering temperature of the R sublattice caused by weak R–R interactions. In the compound of interest, YbFe_6Ge_6 , resonant x-ray Bragg diffraction can distinguish Fe from Yb (Yb^{3+} , $4f^{13}$) magnetism by tuning the x-ray energy to an Fe atomic resonance. Iron moments align with the kagome plane in a spontaneous transition at ≈ 63 K. They adopt a collinear antiferromagnetic structure depicted in Fig. 2, which belongs to an orthorhombic magnetic crystal class that includes anti-inversion ($\bar{1}$) [4].

Anti-inversion among the elements of symmetry in a magnetic crystal class exerts a profound influence on diffraction amplitudes. For Bragg diffraction of x-rays enhanced by an atomic resonance, charge, and magnetic contributions to scattering amplitudes are in phase. Moreover, coupling to helicity in primary x-rays is forbidden, with no difference in the intensity of a Bragg spot observed with opposite handed x-rays.

In contrast, anti-inversion invariance imposes a 90° phase shift between nuclear and magnetic contributions in neutron scattering, and they are in quadrature in the intensity of a Bragg spot. A corollary is that the classical polarized neutron diffraction technique, using a departure from unity of the ratio of intensities for primary neutron beams of opposite polarization, is not available for compounds that present a linear magnetoelectric effect. In their measurement of the magnetization distribution in historically important Cr_2O_3 , Brown *et al.* exploited spherical neutron polarimetry [5].

Our symmetry informed diffraction patterns for the resonant x-ray [6] and magnetic neutron [7] diffraction by YbFe_6Ge_6 expose electronic correlations that can be confronted with simulations. Dipoles in resonant x-ray diffraction at the atomic K edge using a parity-even absorption event are proportional to the orbital angular momentum of the resonant ion. Quadrupoles are charginelike (nonmagnetic Templeton-Templeton scattering) and their angular anisotropy reveals the spatial symmetry of the crystal environment. Parity-odd and time-odd (Dirac) multipoles are compulsory in our diffraction amplitudes, because Fe ions use Wyckoff positions in the magnetic structure that are not centers of inversion symmetry [6,7]. Diffraction patterns for the resonant x-ray and magnetic neutron diffraction by Fe ions in YbFe_6Ge_6 are predicted to include anapoles (Dirac dipoles), space-spin correlations, and Dirac quadrupoles familiar in high- T_c ceramic superconductors [7]. To help make the main body of the paper accessible many mathematical details reside in two appendices.

II. CRYSTAL AND MAGNETIC STRUCTURES

Iron moments in YbFe_6Ge_6 depart from the c axis in P6/m'm'm' (No. 191.241, Fig. 1 [8]) in a spontaneous tran-

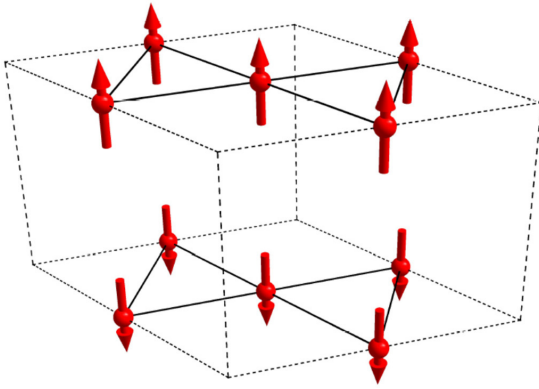


FIG. 1. Collinear antiferromagnetic order of iron dipole moments in YbFe_6Ge_6 at room temperature. Hexagonal magnetic space group $P6/m'm'm'$ (No. 191.241, BNS), and PT-symmetric magnetic crystal class $6/m'm'm'$.

sition at a temperature ≈ 63 K. Iron ions occupy Wyckoff positions (8m) and (4l) that are not centers of inversion symmetry in the orthorhombic space group Cm'mm , with cell dimensions $a \approx 8.828 \text{ \AA}$, $b \approx 5.097 \text{ \AA}$, $c \approx 8.092 \text{ \AA}$ [4], and a basis $\{(1, 2, 0), (-1, 0, 0), (0, 0, 1)\}$ relative to hexagonal (a_h, b_h, c_h) . Axial dipoles are always collinear in the (4l) position and allowed to be noncollinear in (8m). Reflection vectors for hexagonal and orthorhombic structures are labeled (H_0, K_0, L_0) and (h, k, l) , respectively, with $h = H_0 + 2K_0$, $k = -H_0$, $l = L_0$. The orthorhombic structure belongs to the centrosymmetric magnetic crystal class $m'mm$, and anti-inversion ($\bar{1}$) is among the elements of symmetry (identical to properties of $6/m'm'm'$ in Fig. 1). Kerr rotation [9] and the piezomagnetic effect are not permitted by $m'mm$. In the following analysis of diffraction patterns, Fe multipoles specified in Appendices A and B are referred to orthogonal vectors labeled (ξ, η, ζ) derived from the orthorhombic unit cell depicted in Fig. 2.

III. RESONANT X-RAY DIFFRACTION

Our resonant x-ray diffraction amplitudes are derived from universal expressions [6] and an electronic structure factor Eq. (A1). In line with current practice, primary photon polarizations labeled σ and π are perpendicular and parallel to the

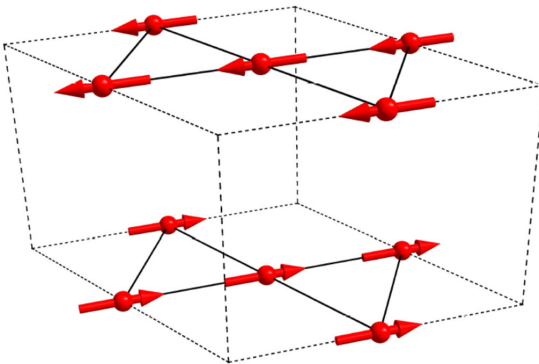


FIG. 2. PT-symmetric orthorhombic configuration of iron dipole moments in YbFe_6Ge_6 at a low temperature < 63 K. Magnetic space group Cm'mm (No. 65.483, BNS).

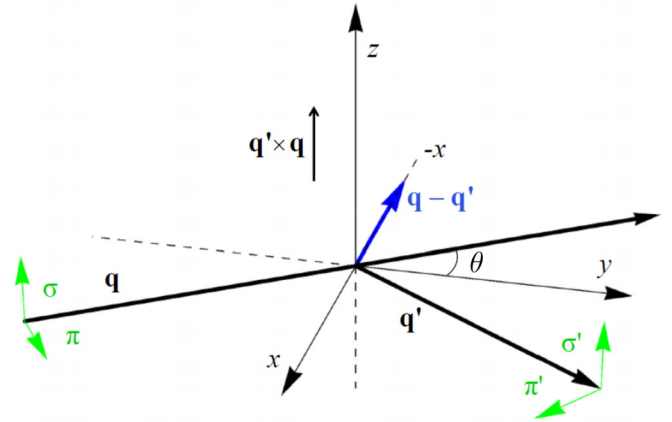


FIG. 3. Primary (σ, π) and secondary (σ', π') states of polarization. Corresponding wave vectors $\mathbf{q}$ and $\mathbf{q}'$ subtend an angle 2θ . The Bragg condition for diffraction is met when $\mathbf{q} - \mathbf{q}'$ coincides with a reflection vector (h, k, l) of the orthorhombic reciprocal lattice. Crystal vectors that define local axes (ξ, η, ζ) and the depicted Cartesian (x, y, z) coincide in the nominal setting of the crystal.

plane of scattering, respectively, and secondary polarization carry a prime as in Fig. 3. Regarding diffraction amplitudes, $(\pi'\sigma)$ and $(\sigma'\sigma)$ apply to primary σ polarization rotated to the π channel and returned to the σ channel, respectively. In the diffraction setting crystals are rotated around the reflection vector by an angle ψ (an azimuthal angle scan).

Valence states accessed by photoejected electrons interact with neighboring ions when x-rays excite a core resonance. Thus, electronic multipoles in the ground state observed in diffraction are rotationally anisotropic with a symmetry corresponding to the position symmetry of the resonant ion. Absence conditions in Bragg diffraction can be violated by relatively weak spots arising from nonspherical atomic charge (Templeton-Templeton scattering) [10]. Tuning the energy of x-rays to an atomic resonance has two obvious benefits. In the first place, there is a welcome enhancement of Bragg spot intensities and, secondly, spots are element specific. There are four scattering amplitudes labeled by photon polarization, two with unrotated and two with rotated states of polarization [6]. Strong Thomson scattering, by spherically symmetric atomic charge, that overwhelms weak signals is absent in rotated channels of polarization. It is allowed in unrotated channels of polarization using a parity-even absorption, but absent in a parity-odd absorption, e.g., electric dipole-electric dipole (E1-E1) and electric dipole - electric quadrupole (E1-E2) events. Schmitt *et al.* [11] review experimental advantages in measuring rotated scattering amplitudes $(\pi'\sigma)$.

The Laue condition for diffraction requires a consideration of the cell dimensions and the energy of an atomic absorption event. The Bragg angle θ in Fig. 3 is determined by $\sin(\theta) = (\lambda/2c)$ for a reflection $(0, 0, l)$, say, with the photon wavelength $\lambda \approx (12.4/E) \text{ \AA}$ and E in units of keV. Iron $L_{2,3}$ edges are at energies $E \approx 0.71$ keV, and the Laue condition is not satisfied by Miller indices of immediate interest. Henceforth, we consider the iron K edge with $E \approx 7.115$ keV that accesses $4p$ (E1) and $3d$ (E2) valence states [6].

Iron multipoles $\langle O_Q^K \rangle$ of rank K and $(2K + 1)$ projections in the interval $-K \leq Q \leq K$ are used to formulate bulk

TABLE I. Angular brackets about a spherical electronic tensor in a generic multipole $\langle O_Q^K \rangle$ denote an expectation value, or time-average. Parity (σ_π) and time (σ_θ) signatures = ± 1 , e.g., $\langle t_Q^K \rangle$ for magnetic neutron diffraction is parity-even ($\sigma_\pi = +1$) and time-odd ($\sigma_\theta = -1$). Iron ions in YbFe_6Ge_6 occupy acentric Wyckoff positions, and Dirac multipoles $\langle g_Q^K \rangle$ and $\langle G_Q^K \rangle$ with $\sigma_\theta = \sigma_\pi = -1$ are permitted. Operator equivalents are found in Appendix B and Refs. [7,12].

Signature	σ_π	σ_θ
<i>Neutrons</i>		
$\langle t_Q^K \rangle$	+1	-1
$\langle g_Q^K \rangle$	-1	-1
<i>Photons</i>		
$\langle T_Q^K \rangle$	+1	$(-1)^K$
$\langle G_Q^K \rangle$	-1	-1

properties, e.g., dichroic signals, and Bragg diffraction patterns [6,7]. Angular brackets about the spherical tensor operator denote a time-average (expectation value), i.e., multipoles are properties of the electronic ground-state. Table I contains the discrete symmetries of electronic multipoles in amplitudes for resonant x-ray and magnetic neutron diffraction [6,7]. A multipole must respect site symmetries, according to Neumann's principle, and restrictions on projections Q that flow from it are given in Appendix A. The range of values of the multipole rank K is fixed by the triangle rule, and $K = 0 - 2$, $K = 1 - 3$ and $K = 0 - 4$ for E1-E1, E1-E2 and E2-E2 events, respectively.

Parity-even ($\sigma_\pi = +1$) diffraction amplitudes E1-E1 and E2-E2 incorporate a time signature $\sigma_\theta(-1)^K = +1$ [6], whereupon electronic structure factors Eqs. (A2) and (A3) are zero, to an excellent approximation, for Miller indices odd l and even K . The corresponding $(\sigma'\sigma)$ amplitude for an E1-E1 event is zero, because it does not contain dipoles $K = 1$, unlike $(\sigma'\sigma)$ for an E2-E2 event [6]. Amplitudes for Wyckoff positions (8m) and (4l) are identical for even k apart from a numerical factor. For a reflection $(0, k, l)$ with $k = 2n$, $l = (2m + 1)$ and an E1-E1 absorption event (trivial numerical factors are omitted in Eqs. (1)–(4),

$$(\pi'\sigma) = \langle T_{+1}^1 \rangle'' [\sin(\theta) \cos(\beta) - \cos(\theta) \sin(\beta) \sin(\psi)], \quad (1)$$

with $\cos(\beta) = -k/[k^2 + (bl/c)^2]^{1/2}$. The Fe dipole moment parallel to the a_h axis, $\langle T_{+1}^1 \rangle'' \propto \langle T_\eta^1 \rangle$, is observed. For absorption at a K edge, axial dipoles are proportional to the orbital angular momentum of the resonant ion, and this property of resonant x-ray scattering is visited in Sec. V. The azimuthal angle ψ measures rotation of the crystal sample about the reflection vector $(0, k, l)$, and the orthorhombic ξ axis and the y axis in Fig. 3 are parallel for $\psi = 0$.

The corresponding unrotated amplitude $(\pi'\pi)$ for $(0, k, l)$ is found to be purely real. Thus, all four amplitudes are purely real (recall that $(\sigma'\sigma) = 0$), and intensity of a Bragg spot is not influenced by circular polarization (helicity) in the primary x-ray beam. The quantity of interest in this regard is a chiral signature $\{(\sigma'\pi)^*(\sigma'\sigma) + (\pi'\pi)^*(\pi'\sigma)\}''$ that measures

the response of a Bragg spot to circular polarization in the primary beam [10]; a null value holds for all considered reflections.

Templeton-Templeton scattering in an E1-E1 event is provided by the quadrupoles $\langle T_Q^2 \rangle$ with projections $Q = 0, \pm 2$. Setting $l = 0$ and using odd h, k with $(h + k) = 2n$ in $(h, k, 0)$, for example, one finds,

$$\begin{aligned} (\pi'\sigma)(8m) &= \sin(\psi) \langle T_{+2}^2 \rangle'' [\sin(\theta) \cos(\psi) \sin(2\chi) \\ &\quad - \cos(\theta) \cos(2\chi)], \\ (\pi'\sigma)(4l) &= \sin(\theta) \sin(2\psi) [\sqrt{6} \langle T_0^2 \rangle + 2 \cos(2\chi) \langle T_{+2}^2 \rangle'] \\ &\quad + 4 \cos(\theta) \sin(\psi) \sin(2\chi) \langle T_{+2}^2 \rangle'. \end{aligned} \quad (2)$$

Diffraction amplitudes (8m) and (4l) are proportional to $\sin(\psi)$, but otherwise very different functions of the azimuthal angle. The relations $\Psi_Q^K(8m) = -\Psi_{-Q}^K(8m)$ and $\Psi_Q^K(4l) = \Psi_{-Q}^K(4l)$ for odd k are responsible for the differences. Thus, $(\pi'\sigma)(8m)$ is conventional Templeton-Templeton scattering expected at a forbidden reflection with odd h . In Eq. (2), $\cos(\chi) = -[h/\sin(\theta)](\lambda/2a)$, and ζ and z axes are parallel at $\psi = 0$. Amplitudes $(\pi'\sigma)(8m)$ and $(\pi'\sigma)(4l)$ for $(h, k, 0)$ and even h, k possess identical structures, namely, $(\pi'\sigma)(4l)$ in Eq. (2).

Wyckoff positions (8m) and (4l) are not centers of inversion symmetry and Dirac multipoles $\langle G_Q^K \rangle$ in Table I are compulsory, and they contribute in diffraction using a parity-odd E1-E2 absorption event. Operator equivalents for $\langle G_Q^K \rangle$ are presented in Ref. [12]. With $\sigma_\pi = \sigma_\theta = -1$, structure factors Eqs. (A2) and (A3) are zero for odd l . Notably, $\Psi_{-Q}^K(8m) = [(-1)^{K+k} \Psi_Q^K(8m)]$, whereas $\Psi_{-Q}^K(4l) = [(-1)^K \Psi_Q^K(4l)]$. Anapoles, or Dirac dipoles, $\langle G^1 \rangle$ contribute to bulk properties ($h = k = l = 0$) with $\Psi_{+1}^1(8m) \propto \langle G_{+1}^1 \rangle'$, and likewise for $\Psi_{+1}^1(4l)$. Notably, anapoles contribute to diffraction in the unrotated channel $(\sigma'\sigma)$; no magnetic multipoles contribute to the same channel for diffraction enhanced by an E1-E1 event. Using odd h, k with $(h + k) = 2n$ in $(h, k, 0)$,

$$\begin{aligned} (\sigma'\sigma)(8m) &= \cos(\chi) \cos(\theta) \cos(\psi) \\ &\quad \times [\langle G_{+1}^1 \rangle'' + (1/3)\sqrt{5} \langle G_{+1}^2 \rangle'] + \dots \end{aligned} \quad (3)$$

Contributions to $(\sigma'\sigma)$ are truncated at the level of quadrupoles, and contributions from two remaining octupoles $\langle G_{+1}^3 \rangle''$ and $\langle G_{+3}^3 \rangle''$ are available from Ref. [6]. As expected, amplitudes $(\sigma'\sigma)(8m)$ and $(\sigma'\sigma)(4l)$ are not the same; e.g., the former contains $\langle G_{+1}^1 \rangle'' \propto \langle G_\eta^1 \rangle$ and the latter contains $\langle G_{+1}^1 \rangle' \propto \langle G_\xi^1 \rangle$. Specifically,

$$\begin{aligned} (\sigma'\sigma)(4l) &= \sin(\chi) \cos(\theta) \cos(\psi) \\ &\quad \times [\langle G_{+1}^1 \rangle' - (1/3)\sqrt{5} \langle G_{+1}^2 \rangle''] + \dots, \end{aligned} \quad (4)$$

and, like $(\sigma'\sigma)(8m)$, it is an even function of ψ . The factor $[\cos(\theta) \cos(\psi)]$ in Eqs. (3) and (4) is replaced by $[\sin(2\theta) \sin(\psi)]$ in the amplitude in the rotated channel of polarization

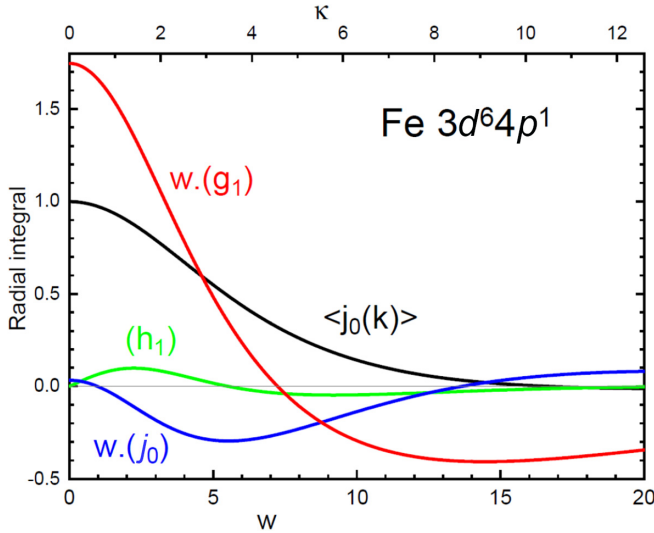


FIG. 4. Radial integrals for an Fe ion displayed as a function of the magnitude of the reflection vector $\kappa = 4\pi s$ with $s = \sin(\theta)/\lambda(\text{\AA}^{-1})$, Bragg angle θ as in Fig. 3, and neutron wavelength λ . Also, $w = 3a_0\kappa$ where a_0 is the Bohr radius. Standard radial integral $\langle j_0(\kappa) \rangle$ in black appears in the axial dipole Eq. (B2). Red, green and blue curves radial integrals in the polar dipole Eq. (B3), with the orbital-spin radial integral (h_1) depicted in green. Radial integrals (g_1) and (j_0) diverge in the forward direction of scattering. Displayed quantities include a factor w , to give $w.(g_1)$ and $w.(j_0)$ that behave nicely for $\kappa \rightarrow 0$. Calculations and figure by van der Laan.

$(\pi'\sigma)$, and it contains one additional quadrupole derived from $\langle G_{+1}^2 \rangle = [\langle G_{+1}^2 \rangle' + i\langle G_{+1}^2 \rangle'']$.

IV. MAGNETIC NEUTRON DIFFRACTION

A dependence of the magnetic neutron scattering amplitude on both the magnitude and direction of the reflection vector κ is a most valuable property of the technique. It enables the measurement of the magnetization density, or its spatial Fourier transform more correctly. The dependence of amplitudes on the magnitude of the reflection vector appears in radial integrals illustrated in Fig. 4. In particular, radial integrals (h_1) and $\langle j_2(\kappa) \rangle$ are derived from spherical Bessel functions of orders 1 and 2, respectively, and the maximum of $\langle j_2(\kappa) \rangle$ occurs at $\kappa \approx 6 \text{\AA}^{-1}$. Dirac and axial quadrupoles are $\langle g^2 \rangle \propto [(h_1)\{\mathbf{S} \otimes \mathbf{n}\}^2]$ and $\langle t^2 \rangle \propto [\langle j_2(\kappa) \rangle \{(\mathbf{S} \times \mathbf{n})\mathbf{n}\}]$ [7]. The cited operator equivalents are reviewed in Appendix B. Suffice to mention that they engage electronic variables spin ($\mathbf{S}$), position ($\mathbf{n}$), and the Zel'dovich anapole ($\mathbf{S} \times \mathbf{n}$). Higher-order axial $\langle t^K \rangle$ ($\sigma_\theta = -1$, $\sigma_\pi = +1$) and polar $\langle g^K \rangle$ ($\sigma_\theta = \sigma_\pi = -1$) multipoles are not included in the present study. Intensity of a Bragg spot is $|\langle \mathbf{Q}_\perp \rangle|^2 = |\langle \mathbf{Q} \rangle|^2 - |\langle \mathbf{e} \cdot \langle \mathbf{Q} \rangle| |^2$, with a unit vector $\mathbf{e} = (\kappa/\kappa)$. In general, $\langle \mathbf{Q} \rangle = [\langle \mathbf{Q} \rangle^{(+)} + \langle \mathbf{Q} \rangle^{(-)}]$, where superscripts label axial $(+)$ and polar $(-)$ intermediate amplitudes. The dipole approximation for Bragg diffraction derived by Schwinger $\langle \mathbf{Q} \rangle^{(+)} = (1/2)\langle \mu \rangle$ uses $\langle j_0(\kappa) \rangle = 1$ for $\kappa \rightarrow 0$, and a magnetic moment $\langle \mu \rangle = \langle 2\mathbf{S} + \mathbf{L} \rangle$.

Neutron scattering amplitudes for Wyckoff positions (8m) and (4l) are derived from electronic structure factors Eqs. (A2) and (A3), respectively. Amplitudes are purely imaginary,

as expected for a PT-symmetric magnetic crystal class. In consequence, magnetic and nuclear amplitudes are 90° out of phase and their contributions to the intensity of a Bragg spot are in quadrature, namely, total intensity = $[\langle \mathbf{Q}_\perp \rangle]^2 + \text{nuclear intensity}$. Projections $\mathbf{Q}$ on multipoles are odd integers since all multipoles are time-odd. In consequence, the Miller index $l = (2m + 1)$ for axial ($\sigma_\pi = +1$) magnetic multipoles, cf. measured diffraction patterns reported in Fig. S18 [4], and $l = 2m$ for polar ($\sigma_\pi = -1$) multipoles. The condition $(h + k) = 2n$ satisfies centering in the magnetic space group.

Wyckoff position (8m) and even k , with a common factor $i8(-1)^{m+n}$.

$$\begin{aligned} \langle \mathbf{Q}_\xi \rangle^{(+)} &\approx -e_\xi e_\eta \langle t_{+1}^2 \rangle', \\ \langle \mathbf{Q}_\eta \rangle^{(+)} &\approx -(3/\sqrt{2}) \langle t_{+1}^1 \rangle'' + (e_\xi^2 - e_\zeta^2) \langle t_{+1}^2 \rangle', \\ \langle \mathbf{Q}_\zeta \rangle^{(+)} &\approx e_\eta e_\zeta \langle t_{+1}^2 \rangle'. \end{aligned} \quad (5)$$

For odd k ,

$$\begin{aligned} \langle \mathbf{Q}_\xi \rangle^{(+)} &\approx -(3/\sqrt{2}) \langle t_{+1}^1 \rangle' - (e_\eta^2 - e_\zeta^2) \langle t_{+1}^2 \rangle'', \\ \langle \mathbf{Q}_\eta \rangle^{(+)} &\approx -e_\xi e_\eta \langle t_{+1}^2 \rangle'', \\ \langle \mathbf{Q}_\zeta \rangle^{(+)} &\approx e_\xi e_\zeta \langle t_{+1}^2 \rangle''. \end{aligned} \quad (6)$$

Observed axial dipoles $\langle \mathbf{t}^1 \rangle$ represented by Eq. (B2) are parallel to the η and ξ axes, respectively. Quadrupoles $\langle t_{+1}^2 \rangle = [\langle t_{+1}^2 \rangle' + i\langle t_{+1}^2 \rangle'']$, significant at large reflection vectors $\kappa \approx 6 \text{\AA}^{-1}$, are seen to contribute to all diffraction amplitudes.

Wyckoff position (4l) and all k , and a common factor $[i4(-1)^{m+k}]$. Otherwise, $\langle \mathbf{Q} \rangle^{(+)}$ is identical to (8m) with even k .

Polar multipoles need even $l = 2m$. The anapole $\langle \mathbf{g}^1 \rangle$ is represented by Cartesian components of $\langle \mathbf{D} \rangle$ defined in Eq. (B3). Observed anapoles are $\langle \mathbf{D}_\xi \rangle$ and $\langle \mathbf{D}_\eta \rangle$ for even and odd k , respectively. For Wyckoff positions (8m) and even k , with a common factor $[i8(-1)^{m+n}]$,

$$\begin{aligned} \langle \mathbf{Q}_{\perp,\xi} \rangle^{(-)} &\approx 2e_\xi e_\eta e_\zeta \langle g_{+1}^2 \rangle'', \\ \langle \mathbf{Q}_{\perp,\eta} \rangle^{(-)} &\approx e_\zeta [\langle \mathbf{D}_\xi \rangle + (2e_\eta^2 - 1) \langle g_{+1}^2 \rangle''], \\ \langle \mathbf{Q}_{\perp,\zeta} \rangle^{(-)} &\approx e_\eta [-\langle \mathbf{D}_\xi \rangle + (2e_\zeta^2 - 1) \langle g_{+1}^2 \rangle'']. \end{aligned} \quad (7)$$

In particular, $\langle \mathbf{Q}_\perp \rangle^{(-)} = (0, 0, \langle \mathbf{Q}_{\perp,\zeta} \rangle^{(-)})$ for $l = 0$. The corresponding results for odd k are,

$$\begin{aligned} \langle \mathbf{Q}_{\perp,\xi} \rangle^{(-)} &\approx e_\zeta [-\langle \mathbf{D}_\eta \rangle + (2e_\xi^2 - 1) \langle g_{+1}^2 \rangle'], \\ \langle \mathbf{Q}_{\perp,\eta} \rangle^{(-)} &\approx 2e_\xi e_\eta e_\zeta \langle g_{+1}^2 \rangle', \\ \langle \mathbf{Q}_{\perp,\zeta} \rangle^{(-)} &\approx e_\xi [\langle \mathbf{D}_\eta \rangle + (2e_\zeta^2 - 1) \langle g_{+1}^2 \rangle']. \end{aligned} \quad (8)$$

Notably, Dirac quadrupoles $\langle g_{+1}^2 \rangle''$ and $\langle g_{+1}^2 \rangle'$ are present in all components of the polar amplitudes. Amplitudes for Wyckoff position (4l) and all k , have a common factor $[i4(-1)^{m+k}]$. Otherwise, $\langle \mathbf{Q}_\perp \rangle^{(-)}$ is identical to (8m) amplitudes in Eq. (7) with even k .

V. CONCLUSIONS

There is currently no direct evidence that the magnetic structure of the kagome metal YbFe_6Ge_6 is P(parity)/T(time)-symmetric [4]. Neutron polarization analysis was not used by Yao *et al.* to verify the symmetry. Furthermore, the distribution of Fe magnetization and the Fe atomic form factor in YbFe_6Ge_6 is work to be done. Shull has published these measurements for elemental iron, cf. Fig. 2 in Ref. [13]. Likewise, PT-symmetry can be checked by resonant x-ray diffraction. The symmetry guarantees that intensity of a magnetic Bragg spot is independent of circular polarization (helicity) in the primary beam, i.e., intensity is the same for left and right circularly polarized x-rays.

I report symmetry informed calculations of neutron and resonant x-ray diffraction patterns for the collinear antiferromagnetic structure $\text{Cm}'\text{mm}$ inferred from limited neutron Bragg diffraction patterns [4]. A linear magnetoelectric effect is allowed by $\text{Cm}'\text{mm}$, as with historically important chromium sesquioxide, and Kerr rotation [9] and the piezomagnetic effect are not permitted.

PT symmetry in the magnetic structure protects against coupling to neutron polarization. In consequence, the method for neutron polarization analysis used by Shull is not available, but the distribution of iron magnetization can be measured with precision using neutron polarimetry. Shull's data on elemental Fe extends to $s = \sin(\theta)/\lambda = 1.157 \text{ \AA}^{-1}$, and data on PT-symmetric Cr_2O_3 extends to $s = 0.75 \text{ \AA}^{-1}$ [5]. Quadrupoles that are predicted here to exist in the distribution of Fe magnetization are caused by correlations between electronic anapole and position variables. They have optimal values at a smaller wavevector $s \approx 0.50 \text{ \AA}^{-1}$ ($\kappa \approx 6 \text{ \AA}^{-1}$) [Eqs. (5) and (6)] that can be confronted with simulations of the electronic structure [14,15]. Dirac quadrupoles in neutron diffraction amplitudes [Eqs. (7) and (8)] offer a sound interpretation of magnetic neutron diffraction by high- T_c materials [7]. The Dirac quadrupole operator equivalent is made from spin and position variables [7,16]. Results for the radial integral (h_1) presented in Fig. 4 indicate that iron Dirac quadrupoles possess an optimal value for $s \approx 0.16 \text{ \AA}^{-1}$. Axial dipoles, closely related to the magnetic moment Eq. (B2), and anapoles Eq. (B3) contribute to neutron scattering amplitudes presented in Eqs. (5)–(8).

Resonant x-ray Bragg diffraction enhanced by a Fe absorption event has the obvious advantage of distinguishing properties of Fe and Yb ions in YbFe_6Ge_6 . No such experiments are in the literature. Exact scattering amplitudes for space group forbidden reflections reported in Sec. III exploit universal expressions for E1-E1 and E1-E2 amplitudes, where E1 and E2 denote an electric dipole and electric quadrupole, respectively [6]. Enhancement by an E2-E2 event at the iron K edge measures orbital angular momentum that is different for $3d^5$ and $3d^6$ atomic configurations; the former is spherically symmetric and the additional electron in the latter configuration is exposed to the electron-lattice interaction. Relevant E2-E2 diffraction amplitudes are readily calculated from available universal expressions [6]. A null E1-E1 unrotated ($\sigma'\sigma$) amplitude is predicted. Equations (1) and (2) for the rotated channel of polarization demonstrate a dependence of amplitudes on a magnetic dipole and nonmagnetic

quadrupoles (Templeton-Templeton scattering). Anapoles are a main attraction in Eqs. (3) and (4) for Dirac amplitudes ($\sigma'\sigma$) and an E1-E2 event, with Bragg spots predicted to be free of stronger E1-E1 signals. Amplitudes in Eqs. (1)–(4) include the dependence on an azimuthal angle.

To summarize, electronic correlations in conjunction with spin-orbit coupling in crystalline materials create valuable and enigmatic effects [17–19]. These include the magnetoelectric effect, collinear antiferromagnetic order, altermagnetism and so-called hidden orders in which a state of matter exists without an easily detectable order parameter. Scattering techniques often have much to offer in gathering incisive information on properties of solids not available with other experimental methods. Distributions of magnetization in many crystalline materials have been measured on a subatomic scale and compared to state-of-the-art simulations [13,20]. If the periodicity of the magnetic and chemical structures are the same then magnetic and nuclear scattering occur at the same points in reciprocal space and interfere with one another. In favorable cases the polarization dependence of the interference allows accurate determinations of the magnetic amplitude. However, the required interference is not available in PT-symmetric (magnetoelectric) solids because magnetic and nuclear contributions to the scattering amplitude are 90° out of phase. In which case, magnetic and nuclear contributions to the intensity of a Bragg spot are in quadrature. Spherical neutron polarimetry can be applied to such materials, e.g., chromium sesquioxide (Cr_2O_3) [5]. Notably, the expectation value of the quadrupole contribution to the neutron scattering amplitude ($\langle t^2 \rangle$ in Appendix B) vanishes in the extreme limit of an infinite spin-orbit coupling. The quadrupole will be relatively large for negligible spin-orbit coupling required to sustain altermagnetism [18]. The optimum value of $\langle t^2 \rangle$ for iron in YbFe_6Ge_6 will be in the region $\kappa \approx 6 \text{ \AA}^{-1}$. Anapoles (Dirac dipoles) present a hidden order unveiled by resonant x-ray diffraction. Photon charge and magnetic scattering amplitudes for a solid with PT-symmetry are not phase separated, which contrasts with the corresponding magnetic and nuclear amplitudes. As a result, a chiral signature $\{(\sigma'\pi)^*(\sigma'\sigma) + (\pi'\pi)^*(\pi'\sigma)\}'' = 0$, and the helicity (circular polarization) of primary x-rays is not changed by scattering from YbFe_6Ge_6 [10]. Our x-ray amplitudes Eqs. (1) and (2) are created by axial time-odd (magnetic) dipoles and time-even (nonmagnetic) quadrupoles, respectively, and they are both purely real. Altermagnets share some physical properties with YbFe_6Ge_6 , e.g., collinear antiferromagnetism [18]. They differ with respect to the chiral signature, however, for it can be different from zero for an altermagnet where PT-symmetry is absent, e.g., RuO_2 with magnetic symmetry $\text{P2}_1/\text{c}$ (No. 14.75).

A study of V_2O_3 that exploits the signal enhancement provided by the vanadium K-edge absorption event is noted for a full use of linear photon polarization analysis to disentangle multipoles in diffraction amplitudes [21]. A peculiarity of enhancement at the K edge is that spin degrees of freedom in the valence state make no contribution to electronic multipoles. This means that magnetic multipoles for the ferric ion Fe^{3+} ($3d^5$) available in diffraction at the K absorption edge are zero, because the nominal atomic state has zero orbital angular momentum. A detailed study of haematite ($\alpha\text{-Fe}_2\text{O}_3$) showed, beyond reasonable doubt, that magnetic multipoles contribute

to the diffraction pattern, a result that implies unquenched orbital angular momentum in the valence state of the material [22].

ACKNOWLEDGMENTS

Dr. W. Yao endorsed IRs ($\Psi_{15} + \Psi_{16}$) in Table S4 for the low-temperature magnetic structure of YbFe_6Ge_6 , and not IRs ($\Psi_{17} - \Psi_{18}$) stated in the text [4]. Professor R. D. Johnson spotted incorrect IRs, and Dr. D. D. Khalyavin confirmed the magnetic space groups and prepared Figs. 1 and 2. Professor G. van der Laan generated Figs. 3 and 4.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: ELECTRONIC STRUCTURE FACTOR

A universal spherical structure factor of rank K ,

$$\Psi_Q^K = [\exp(i\boldsymbol{\kappa} \cdot \mathbf{d}) \langle \mathbf{O}_Q^K \rangle_{\mathbf{d}}], \quad (\text{A1})$$

determines x-ray and neutron Bragg diffraction amplitudes. The generic electronic multipole $\langle \mathbf{O}_Q^K \rangle$ possesses $(2K+1)$ projections in the interval $-K \leq Q \leq K$. A complex conjugate $\langle \mathbf{O}_Q^K \rangle^* = (-1)^Q \langle \mathbf{O}_{-Q}^K \rangle$. Our phase convention for real and imaginary parts labeled by single and double primes is $\langle \mathbf{O}_Q^K \rangle = [\langle \mathbf{O}_Q^K \rangle' + i \langle \mathbf{O}_Q^K \rangle'']$. Cartesian dipole moments in an orthorhombic cell (ξ, η, ζ) are $\langle \mathbf{O}_\xi^1 \rangle = -\sqrt{2} \langle \mathbf{O}_{+1}^1 \rangle'$, $\langle \mathbf{O}_\eta^1 \rangle = -\sqrt{2} \langle \mathbf{O}_{+1}^1 \rangle''$, and $\langle \mathbf{O}_\zeta^1 \rangle = \langle \mathbf{O}_0^1 \rangle$. Multipole types encountered in resonant x-ray and magnetic neutron diffraction are reviewed in Table I.

Multipoles for resonant x-ray and neutron scattering abide by the same discrete symmetry requirements but they are different in detail. Magnetic neutron multipoles are time-odd, and axial or polar (Dirac) for Wyckoff positions that are not centers of inversion symmetry. Multipoles in resonant x-ray scattering are parity-even for electric dipole-electric dipole (E1-E1) and electric quadrupole-electric quadrupole (E2-E2) absorption events. They are time-even (time-odd) for even (odd) rank K . Parity-odd multipoles are permitted for Wyckoff positions that are not centers of inversion symmetry, and they are either time-even or time-odd. The structure factor Ψ_Q^K is informed of all elements of symmetry in the magnetic space group. In Eq. (A1), the reflection vector $\boldsymbol{\kappa}$ is defined by integer Miller indices (h, k, l) with $(h+k) = 2n$ from a centering condition. The implied sum is over Fe ions in sites $\mathbf{d}$ in a magnetic unit cell. In more detail, Eq. (A1) possesses information about the relevant Wyckoff positions available in the Bilbao table MWYCKPOS for the magnetic symmetry of interest [8]. Site symmetry that might constrain projections Q is given in the same table. Wyckoff positions in a unit cell are related by operations listed in the table MGENPOS [8]. Taken together, the two tables provide all information required to evaluate Eq. (A1) and, thereafter, x-ray and neutron Bragg diffraction amplitudes [6,7].

Evaluated for Wyckoff positions (8m) in the magnetic space group $\text{Cm}'\text{mm}$ (No. 65.483),

$$\Psi_Q^K(8m) = 2(-1)^n [\exp(i\varphi) + \sigma_\pi(-1)^Q \exp(-i\varphi)] \times [\langle \mathbf{O}_Q^K \rangle + \sigma_\pi(-1)^k (-1)^{K+Q} \langle \mathbf{O}_{-Q}^K \rangle], \quad (\text{A2})$$

where $\varphi = 2\pi/z$. We use a general coordinate $z = 1/4$ [4]. In Eq. (A2), σ_π and σ_θ are signatures of discrete symmetries of parity and time, respectively, with $\sigma_\pi = +1$ (-1) for axial (polar) and $\sigma_\theta = +1$ (-1) for time-even (time-odd, magnetic). Site symmetry (8m) demands $\sigma_\theta(-1)^Q = +1$ and no more. Site symmetry for Wyckoff positions (4l) is sturdier with a structure factor,

$$\Psi_Q^K(4l) = 2(-1)^k \langle \mathbf{O}_Q^K \rangle [\exp(i\varphi) + \sigma_\pi(-1)^Q \exp(-i\varphi)]. \quad (\text{A3})$$

The electronic multipole in Eq. (A3) satisfies $\langle \mathbf{O}_Q^K \rangle = [\sigma_\theta \sigma_\pi (-1)^K \langle \mathbf{O}_{-Q}^K \rangle]$ in addition to $\sigma_\theta(-1)^Q = +1$. Multipoles for parity-even E1-E1 and E2-E2 absorption events possess a time signature $\sigma_\theta(-1)^K = +1$.

APPENDIX B: NEUTRON OPERATOR EQUIVALENTS

An intermediate operator $\mathbf{Q}$ for magnetic neutron scattering by electrons can be taken to be [7],

$$\mathbf{Q} = \exp(i\mathbf{R}_j \cdot \boldsymbol{\kappa}) [\mathbf{s}_j - (i/\hbar\kappa^2) (\mathbf{e} \times \mathbf{p}_j)]. \quad (\text{B1})$$

Here, $\mathbf{R}_j$, $\mathbf{s}_j$, and $\mathbf{p}_j$ are operators for electron position, spin and linear momentum, respectively. The unit vector $\mathbf{e} = (\boldsymbol{\kappa}/\kappa)$. The amplitude of magnetic neutron Bragg diffraction $\langle \mathbf{Q}_\perp \rangle = [\mathbf{e} \times (\mathbf{Q} \times \mathbf{e})]$ yields an intensity $|\langle \mathbf{Q}_\perp \rangle|^2 = |\langle \mathbf{Q} \rangle|^2 - |(\mathbf{e} \cdot \langle \mathbf{Q} \rangle)|^2$. Note that $\mathbf{Q}$ is arbitrary to within a scalar function proportional to the reflection vector $\boldsymbol{\kappa}$.

The dipole approximation for Bragg diffraction derived by Schwinger is $\langle \mathbf{Q} \rangle^{(+)} \approx (1/2) \langle \boldsymbol{\mu} \rangle$ with a magnetic moment $\langle \boldsymbol{\mu} \rangle = \langle 2\mathbf{S} + \mathbf{L} \rangle$ [7]. A useful approximation to the axial dipole $\langle \mathbf{t}^1 \rangle$ uses a gyromagnetic ratio g for an orbital contribution $\langle \mathbf{L} \rangle \propto (g-2) \langle \mathbf{S} \rangle$,

$$\langle \mathbf{t}^1 \rangle \approx (\langle \boldsymbol{\mu} \rangle / 3) [\langle j_0(\kappa) \rangle + \langle j_2(\kappa) \rangle (g-2)/g]. \quad (\text{B2})$$

The radial integral $\langle j_0(\kappa) \rangle$ is illustrated in Fig. 4. Even rank multipoles arise from correlations between anapole and position $\mathbf{n} = \mathbf{R}/R$ variables that are probed in the orbital-spin contribution to $\langle \mathbf{Q} \rangle^{(+)}$. Specifically, a quadrupole operator equivalent $\mathbf{t}^2 \propto [\langle j_2(\kappa) \rangle \{(\mathbf{S} \times \mathbf{n})\mathbf{n}\}]$, where $(\mathbf{S} \times \mathbf{n})$ is the operator for a spin anapole. As for the radial integral, $\langle j_2(0) \rangle = 0$ and the maximum of $\langle j_2(\kappa) \rangle$ occurs at $\kappa \approx 6 \text{ \AA}^{-1}$.

In general $\langle \mathbf{Q} \rangle = [\langle \mathbf{Q} \rangle^{(+)} + \langle \mathbf{Q} \rangle^{(-)}]$, where a polar contribution $\langle \mathbf{Q} \rangle^{(-)}$ is essential for magnetic ions at acentric Wyckoff positions. A polar dipole $\langle \mathbf{D} \rangle$ depends on three radial integrals illustrated in Fig. 4. We use,

$$\langle \mathbf{D} \rangle = (1/2) [i(g_1) \langle \mathbf{n} \rangle + 3(h_1) \langle \mathbf{S} \times \mathbf{n} \rangle - (j_0) \langle \boldsymbol{\Omega} \rangle], \quad (\text{B3})$$

and an orbital anapole $\langle \boldsymbol{\Omega} \rangle = [(\mathbf{L} \times \mathbf{n}) - (\mathbf{n} \times \mathbf{L})]$. Radial integrals (g_1) and (j_0) diverge in the forward direction of

scattering ($\kappa \rightarrow 0$). We appeal to the orbital-spin contribution to $\langle \mathbf{Q} \rangle^{(-)}$ for an approximation to the polar quadrupole. It is proportional to $\langle h_1 \rangle$ at the chosen level of working, as in Eq. (B3), and arrive at,

$$\langle \mathbf{Q} \rangle^{(-)} \approx i(\mathbf{e} \times \langle \mathbf{D} \rangle) - i\sqrt{3}\{\mathbf{e} \otimes \langle \mathbf{H} \rangle^2\}^1, \quad (\text{B4})$$

with a quadrupole operator equivalent,

$$\mathbf{H}^2 = \sqrt{5}(h_1)\{\mathbf{S} \otimes \mathbf{n}\}^2. \quad (\text{B5})$$

Tensor products in Eqs. (B4) and (B5) follow a standard definition for two spherical tensors of ranks a and b , namely,

$$\{\mathbf{A}^a \otimes \mathbf{B}^b\}_Q^K = A_\alpha^a B_\beta^b (a\alpha b\beta | KQ), \quad (\text{B6})$$

with a sum over repeated indices α, β . The Clebsch-Gordan coefficient in Eq. (B6) can be defined in terms of a 3j-symbol,

$$(a\alpha b\beta | KQ) = (-1)^{-a+b-Q} \sqrt{(2K+1)} \begin{pmatrix} a & b & K \\ \alpha & \beta & -Q \end{pmatrix}. \quad (\text{B7})$$

-
- [1] T. Mazet and B. J. Malaman, Evidence of spin reorientation in YbFe₆Ge₆ from neutron diffraction and ⁵⁷Fe Mössbauer experiments, *J. Phys.: Condens. Matter* **12**, 1085 (2000).
- [2] M. A. Avila, T. Takabatake, Y. Takahashi, S. L. Bud'ko, and P. C. Canfield, Direct observation of Fe spin reorientation in single-crystalline YbFe₆Ge₆, *J. Phys.: Condens. Matter* **17**, 6969 (2005).
- [3] J. M. Cadogan and D. H. Ryan, A study on the magnetic behaviour of polymorphic YbFe₆Ge₆, *J. Phys.: Condens. Matter* **22**, 016009 (2010).
- [4] W. Yao *et al.*, Anomalous electrical transport in the kagome magnet YbFe₆Ge₆, *Phys. Rev. Lett.* **134**, 186501 (2025).
- [5] P. J. Brown, J. B. Forsyth, E. Lelièvre-Berna, and F. Tasset, Determination of the magnetization distribution in Cr₂O₃ using spherical neutron polarimetry, *J. Phys.: Condens. Matter* **14**, 1957 (2002).
- [6] V. Scagnoli and S. W. Lovesey, Analysis of azimuthal-angle scans in resonant x-ray Bragg diffraction and parity even and odd atomic multipoles in the multiferroic modification of the terbium manganate TbMnO₃, *Phys. Rev. B* **79**, 035111 (2009).
- [7] S. W. Lovesey and D. D. Khalyavin, Neutron scattering by Dirac multipoles, *J. Phys.: Condens. Matter* **29**, 215603 (2017).
- [8] We use the Belov-Neronova-Smirnova [BNS] setting of magnetic space groups, see Bilbao Crystallographic server, <http://www.cryst.ehu.es>.
- [9] J. Orenstein, Optical nonreciprocity in magnetic structures related to high-T_c superconductors, *Phys. Rev. Lett.* **107**, 067002 (2011).
- [10] J. Fernández-Rodríguez, S. W. Lovesey, and J. A. Blanco, Polarization analysis in resonant x-ray Bragg diffraction by K₂CrO₄ at the Cr K-edge, *Phys. Rev. B* **77**, 094441 (2008).
- [11] A. T. Schmitt, Y. Joly, K. S. Schulze, B. Marx-Glowna, I. Uschmann, B. Grabiger, H. Bernhardt, R. Loetzsch, A. Juhin, and J. Debray, Disentangling x-ray dichroism and birefringence via high-purity polarimetry, *Optica* **8**, 56 (2021).
- [12] S. W. Lovesey and E. Balcar, A guide to electronic multipoles in photon scattering and absorption, *J. Phys. Soc. Jpn.* **82**, 021008 (2013).
- [13] C. G. Shull and Y. Yamada, Proceedings of the International Conference on Magnetism and Crystallography, Eyoto, 1961 (Phys. Soc. Jpn., 1962); C. G. Shull, *Electronic Structure and Alloy Chemistry of the Transition Elements* (Interscience, New York, 1963), p. 69.
- [14] O. Bunău, A. Y. Ramos, and Y. Joly, *The FDMNES Code in International Tables for Crystallography* (Wiley, New York, 2022), Vol. 1.
- [15] E. N. Ovchinnikova, A. P. Oreshko, and V. E. Dmitrienko, Interference phenomena in X-ray diffraction spectroscopy, *Phys. Usp.* **68**, 393 (2025).
- [16] S. Hayami, Field-induced ferroaxiality in antiferromagnets with magnetic toroidal quadrupole, *Condens. Matter* **10**, 35 (2025).
- [17] L. V. Pourovskii, D. F. Mosca, L. Celiberti, S. Khmelevskiy, A. Paramakanti, and C. Franchini, Hidden orders in spin-orbit-entangled correlated insulators, *Nat. Rev. Mater.* **10**, 674 (2025).
- [18] R. Tamang, S. Gurung, D. P. Rai, S. Brahimi, and S. Lounis, Altermagnetism and altermagnets, *Magnetism* **5**, 17 (2025).
- [19] R. Winkler and U. Zülicke, Standard model of electromagnetism and chirality in crystals, [arXiv:2405.20940](https://arxiv.org/abs/2405.20940).
- [20] P. J. Brown, Magnetization distributions, *Int. J. Mod. Phys. B* **7**, 3029 (1993).
- [21] J. Fernández-Rodríguez, V. Scagnoli, C. Mazzoli, F. Fabrizi, S. W. Lovesey, J. A. Blanco, D. S. Sivia, K. S. Knight, F. de Bergevin, and L. Paolasini, Experimental evidence of anapolar moments in the antiferromagnetic insulating phase of V₂O₃ obtained from x-ray resonant Bragg diffraction, *Phys. Rev. B* **81**, 085107 (2010).
- [22] A. Rodríguez-Fernández, J. A. Blanco, S. W. Lovesey, V. Scagnoli, U. Staub, H. C. Walker, D. K. Shukla, and J. Stremper, Chiral properties of hematite α -Fe₂O₃ inferred from resonant Bragg diffraction using circularly polarized x rays, *Phys. Rev. B* **88**, 094437 (2013).