

Double perovskite $\text{Ba}_2\text{NaOsO}_6$: Magnetic structure, Kramers doublet, and x-ray magnetic dichroic signals

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Of all the oxides of osmium, $\text{Ba}_2\text{NaOsO}_6$ is the only one with a substantial ferromagnetic moment. A fresh theoretical study of the double perovskite is accomplished using a different magnetic symmetry, which embraces all relevant published structural information, and an atomic model of a Kramers doublet formed by the single osmium d electron. It possesses symmetry demanded by the Wyckoff position assigned to Os in a canted ferromagnet. Whereupon, magnetic moments in the paramagnetic and magnetically ordered states of $\text{Ba}_2\text{NaOsO}_6$ are unified. Analytic x-ray magnetic dichroic signals (XMCD) at osmium L_2 and L_3 absorption edges are presented, and shown to agree with hitherto unexplained recent measurements [Agrestini *et al.* *Phys. Rev. Lett.* **133**, 066501 (2024)].

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I. INTRODUCTION

Structural, chemical, and magnetic properties of $\text{Ba}_2\text{NaOsO}_6$ (Os^{7+}) along with $\text{Ba}_2\text{MgReO}_6$ (Re^{6+}) have been studied using various experimental techniques and theoretical methods [1–11]. Among oxides of osmium, including binary OsO_2 and double and triple perovskites, $\text{Ba}_2\text{NaOsO}_6$ is the only one with a substantial ferromagnetic moment in the ordered state [1]. It is substantially larger than in iridates, e.g., Sr_2IrO_4 . Although its single t_{2g} electron orders magnetically, $\text{Ba}_2\text{NaOsO}_6$ shows no evidence of an expected orbital order that causes Jahn-Teller distortion and should destroy its cubic symmetry. The origin of ferromagnetic order is unresolved, and evidently subtle since isostructural, isovalent, and also Mott insulating $\text{Ba}_2\text{LiOsO}_6$ orders antiferromagnetically [4]. Specifically, the requirement of spin-orbit coupling to describe $\text{Ba}_2\text{NaOsO}_6$ makes it a Dirac-Mott insulator [6], and the coupling precludes altermagnetism. In addition, recently reported x-ray magnetic circular dichroism (XMCD) for $\text{Ba}_2\text{NaOsO}_6$ has not been interpreted until now [11]. Signals measured at the two osmium L edges are unusual in that one is zero (L_3), to a good approximation. Moreover, the edge with a null signal is not the one in previous measurements at L edges.

An interpretation of XMCD signals requires the magnetic space group, and drawing on published experimental results we propose Pnn'm' (No. 58.398) for the low temperature magnetic phase of $\text{Ba}_2\text{NaOsO}_6$. The compound forms an orthorhombic magnetic structure depicted in Fig. 1

below a transition temperature ≈ 7 K. Ferromagnetic layers are strongly canted with respect to the neighboring layers. Osmium ions ($5d^1$) occupy Wyckoff positions with low spatial symmetry. Together with a specified Kramers doublet, Pnn'm' leads to satisfactory XMCD signals. Specifically, the L_3 signal can be zero from interference between a component in the ground state quartet and an excited doublet. A calculated Os saturation magnetic moment accords with previous measurements. Calculations of the two mentioned properties reported here make extensive use of Racah algebra and nontrivial XMCD reduced matrix elements.

The chemical structure of $\text{Ba}_2\text{NaOsO}_6$ at room temperature is cubic $\text{Fm}\bar{3}\text{m}$ [1,2]. Da Cruz Pinha Barbosa *et al.* derive the cited long-range magnetic structure from neutron powder diffraction patterns (Fig. 1(d) [9]), and Lu *et al.* exploit NMR to the same end (Fig. 4(d) [7]). Synchrotron x-ray diffraction patterns reveal the chemical and magnetic structures of single crystals of $\text{Ba}_2\text{MgReO}_6$ (Fig. 1(c) [8]). The osmium saturation magnetic moment is small [2], and it would be identically zero if the Kramers doublet was an unspoiled quartet (Eq. (8) [3]). In this case, the ground state is a quartet (total angular momentum $j = 3/2$) with an excited doublet ($j = 1/2$). An atomic model of a Kramers doublet can be useful in reaching a tenable understanding of magnetic properties when covalent bonding is strong [6,11]. It is created from spin-orbital product states (spin = $1/2$, orbital angular momentum = 2) with quantum numbers J, M ($J = 3/2$ and $5/2$). Here, parameters account for osmium $5d$ strongly hybridized with p orbitals that are close in energy [2].

II. MATERIAL PROPERTIES

The magnetic symmetry of $\text{Ba}_2\text{NaOsO}_6$ is inferred from published experimental results [2,7,8,9], in which case, $\text{Ba}_2\text{NaOsO}_6$ and $\text{Ba}_2\text{MgReO}_6$ have identical magnetic

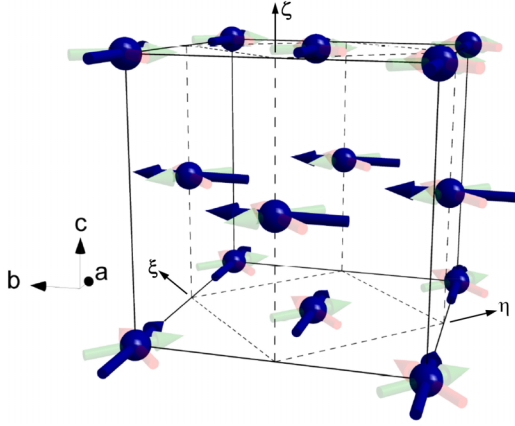


FIG. 1. Ferro- and antiferromagnetic osmium dipole components of the ordered magnetic structure $\text{Ba}_2\text{NaOsO}_6$ are depicted by transparent red and green arrows, respectively. Both the parent cubic [basis (a), (b), (c)] and orthorhombic [basis (ξ , η , ζ)] cells are shown. The basis (ξ , η , ζ) is defined in Appendix A [12].

structures [12]. Osmium ions occupy centrosymmetric sites in orthorhombic $\text{Pnn}'m'$ (No. 58.398 [13]), namely, Wyckoff positions $2a$. The magnetic crystal class $mm'm'$ permits a spontaneous magnetization, and a nonlinear magnetoelectric effect. As anticipated, the cited magnetic symmetry is not compatible with altermagnetism. Magnetic symmetry presented by $\text{Ba}_2\text{NaOsO}_6$ is thoroughly discussed in Appendix A [12]. In summary, a product of a dyad axis of rotation symmetry along the crystal c axis and time reversal symmetries $2'/m'(C_i)$ restricts dipoles to the basal plane. According to ^{23}Na NMR spectra measured and analysed by Lu *et al.* there are two distinct magnetic sites $\text{Na}(\text{Os})$ [7]. The authors appeal to the canted magnetic structure in Fig. 1 for an interpretation of the spectra. This is not a viable interpretation, however, because $\text{Pnn}'m'$ possesses only one suitable magnetic site.

III. ELECTRONIC MULTIPOLES

Neumann's principle places restrictions on osmium electronic multipoles $\langle T_Q^K \rangle$ of rank K and $(2K+1)$ projections in the interval $-K \leq Q \leq K$ used to formulate bulk properties, e.g., dichroic signals, and Bragg diffraction patterns [12,14–16]. Angular brackets about the spherical tensor operator denote a time-average (expectation value), i.e., multipoles are properties of the electronic ground state. A complex conjugate $\langle T_Q^K \rangle^* = (-1)^Q \langle T_{-Q}^K \rangle$. Site symmetry $2'/m'$ for Wyckoff positions $2a$ includes inversion, and invariance of axial multipoles $\langle T_Q^K \rangle$ with respect to the antidyad operation $2'_z$ [13]. It is achieved by imposing the identity $\sigma_\theta(-1)^Q = +1$, where the time signature $\sigma_\theta = +1$ (time even, charginelike) or $\sigma_\theta = -1$ (time odd, magnetic). For $\sigma_\theta = -1$ projections Q are odd, and magnetic dipoles ($K = 1$) are confined to the basal plane. Our phase convention for real and imaginary parts labeled by single and double primes is $\langle T_Q^K \rangle = [\langle T_Q^K \rangle' + i\langle T_Q^K \rangle'']$. A tetragonal cell (ξ , η , ζ) introduced in Appendix A is shown in Fig. 1, with Cartesian dipoles $\langle T_\xi^1 \rangle = -\sqrt{2}\langle T_{+1}^1 \rangle'$ and $\langle T_\eta^1 \rangle = -\sqrt{2}\langle T_{+1}^1 \rangle''$.

XMCD signals are derived from an electronic structure factor Ψ_Q^K defined in Eq. (A1) that presents all relevant magnetic symmetry for osmium ions in $\text{Ba}_2\text{NaOsO}_6$. For bulk magnetic properties,

$$\Psi_Q^K(\text{Pnn}'m') = [\langle T_Q^K \rangle + (-1)^Q \langle T_{-Q}^K \rangle] = 2\langle T_Q^K \rangle'. \quad (1)$$

Symmetry of the Wyckoff position $2a$ requires that the multipole rank and projections Q are such that their sum $(K+Q)$ is even. A spontaneous magnetization is determined by $\Psi_{+1}^1(\text{Pnn}'m') = 2\langle T_{+1}^1 \rangle' = -\sqrt{2}\langle T_\xi^1 \rangle$.

IV. MAGNETIC MOMENTS AND XMCD SIGNALS

Symmetry of Wyckoff positions used by osmium ions requires odd projections Q for a magnetic multipole. In consequence, $[|u\rangle + f|\hat{u}\rangle]$ is a suitable osmium wavefunction, where $|u\rangle$ is a Kramers state, $|\hat{u}\rangle$ its conjugate, and the phase ϕ in $f = \exp(i\phi)$ is to be determined [12,17]. The conjugate (time-reversed) state is constructed with the rule $c|j, m\rangle \rightarrow c^* \{(-1)^{j-m}|j, -m\rangle\}$, where c is a classical number. Using the identity $\langle u|T_Q^K|u\rangle = -\langle \hat{u}|T_Q^K|\hat{u}\rangle$, the corresponding expectation value,

$$\langle T_Q^K \rangle = (1/2) [f\langle u|T_Q^K|\hat{u}\rangle + f^*\langle \hat{u}|T_Q^K|u\rangle], \quad (2)$$

with $f^* = \exp(-i\phi)$. Matrix elements in Eq. (2) are calculated with a standard prescription and known reduced matrix elements (RMEs) [16,18]. Some aspects of the calculations are collected in Appendix B. Regarding the Os atomic wavefunction, spin-orbital product states $\{|\pm 1/2\rangle|l = 2, m\rangle\}$ are rewritten in terms of angular momenta $J = 3/2$ and $J = 5/2$. The Kramers doublet is taken to be

$$|u\rangle = [3/2, 1/2] + t[5/2, -3/2][1 + |t|^2]^{-1/2}, \quad (3)$$

where the mixing parameter t is allowed to be complex. Note that $\langle \hat{u}|T_Q^K|u\rangle$ does not include t^* , and $\langle u|T_Q^K|\hat{u}\rangle$ does not include t . Allowed projections in $\langle u|T_Q^K|\hat{u}\rangle$ are $Q = \pm 1, -3$, and $Q = \pm 1, +3$ for $\langle \hat{u}|T_Q^K|u\rangle$. Atomic quantum numbers J, M in Eq. (3) are the outcome of a search for a minimal model that yields satisfactory paramagnetic and ordered magnetic moments [1,2] and, also, realistic XMCD signals in the ordered phase [11].

A calculation of the magnetic moment $(\mathbf{L} + 2\mathbf{S})$ based on Eq. (3) is outlined in Appendix B. After extensive algebra, one finds

$$\langle (\mathbf{L} + 2\mathbf{S}) \rangle_{+1} = (\sqrt{2}/5) [2f + tf^*\sqrt{3}][1 + |t|^2]^{-1}, \quad (4)$$

with Cartesian components $\langle (\mathbf{L} + 2\mathbf{S})_\xi \rangle = -\sqrt{2}\langle (\mathbf{L} + 2\mathbf{S})_{+1} \rangle'$ and $\langle (\mathbf{L} + 2\mathbf{S})_\eta \rangle = -\sqrt{2}\langle (\mathbf{L} + 2\mathbf{S})_{+1} \rangle''$. A discussion of the results is deferred to the next section.

Measured XMCD signals from $\text{Ba}_2\text{NaCaOsO}_6$ held at a temperature of 3.5 K are shown in Fig. 3 of Ref. [11]. Calculated XMCD signals use RMEs for T^K at L_2 and L_3 edges reported in Appendix B. They employ an axial electric dipole-electric dipole (E1-E1) absorption event [16]. The electronic structure factor Eq. (1) yields the following signals:

$$\begin{aligned} \Psi_{+1}^1(L_2) &= -(1/9) \cos(\phi) [1 + |t|^2]^{-1}, \\ \Psi_{+1}^1(L_3) &= \cos(\phi) [-2 + t9\sqrt{3}](225[1 + |t|^2])^{-1}. \end{aligned} \quad (5)$$

Note that orbital angular momentum ($\mathbf{L}$) obeys a sum rule [14,16],

$$\langle \mathbf{T}^1(\mathbf{L}_2) \rangle + \langle \mathbf{T}^1(\mathbf{L}_3) \rangle = -\langle \mathbf{L} \rangle / (10\sqrt{2}), \quad (6)$$

which can be derived from Eq. (73) in Ref. [16].

V. DISCUSSION AND SUMMARY

XMCD signals Eq. (5) exhibit properties captured in measurements at the L edges of osmium with a sample temperature = 3.5 K [11] (Fig. 3 and Sec. C in the SM, with minimal information about powdered Ba₂NaCaOsO₆ used as a host material). According to the authors, signals measured at osmium L₂ and L₃ absorption edges are of one sign, and the L₃ signal is relatively small; see the text immediately below Fig. 3 in Ref. [11]. According to Eq. (6), XMCD signals of one sign are consistent with a significant orbital moment on the resonant ion. Evidently, the extreme result $\Psi_{+1}^1(\mathbf{L}_3) = 0$ is achieved for a real mixing parameter $t = (2/9\sqrt{3})$ in the Kramers doublet Eq. (3), which then implies that a weak L₃ signal is due to interference of atomic states $J = 3/2$ and $J = 5/2$. The sign of $\Psi_{+1}^1(\mathbf{L}_2)$ is fixed by a single parameter, namely, $\cos(\phi)$. Interestingly, null values of an L₂ signal are known in other materials, including Sr₂IrO₄ [17].

The mixing parameter t in the Kramers doublet Eq. (3) unifies magnetic moments measured in the paramagnetic and ordered phases of Ba₂NaOsO₆ [1,2,11]. A plausible interpretation of the magnetic moment Eq. (4) uses $t = (2/9\sqrt{3})$ that leaves XMCD $\propto \Psi_{+1}^1(\mathbf{L}_3) = 0$. Adding the condition $\langle (\mathbf{L} + 2\mathbf{S}) \rangle_\xi = \langle (\mathbf{L} + 2\mathbf{S}) \rangle_\eta$ yields $\langle (\mathbf{L} + 2\mathbf{S}) \rangle_\xi = 0.546$, which matches the moment measured in the paramagnetic phase. A sample held at about half of the magnetic ordering temperature (Fig. 3(d) in Ref. [11]) possesses a ferromagnetic magnetic moment $\approx 0.2 \mu_B$ [1,2,4]. One achieves $\langle (\mathbf{L} + 2\mathbf{S}) \rangle_\xi = 0.2$ and $\langle (\mathbf{L} + 2\mathbf{S}) \rangle_\eta = 0$ using $t = -0.717$ and $\phi = 0$ in Eq. (4). Corresponding XMCD signals accord with measured signals [11], being of one sign and in a ratio $\{\Psi_{+1}^1(\mathbf{L}_2)/\Psi_{+1}^1(\mathbf{L}_3)\} = 1.90$. The mixing parameter, t , must absorb effects of shielding by electron back-transfer between osmium and neighboring oxygen ions (covalency). Indeed, Gangopadhyay and Pickett [6] claim that the net osmium moment lies primarily on the oxygen ions.

Summarizing, the orthorhombic magnetic space group Pnn'm' (No. 58.398) used to construct Fig. 1 is inferred from the observed canted magnetic structure of Ba₂NaOsO₆ [7,9]. Future measurements of magnetic Bragg diffraction patterns can be confronted with published diffraction patterns for Pnn'm' [12]. The mentioned study includes allowed structural distortions. Down to a sample temperature of 10 K there is no evidence of distortions away from cubic symmetry (neutron powder diffraction patterns [9]). Symmetry of the Wyckoff positions in Pnn'm' imposes restrictions on osmium electronic multipoles. The magnetic structure leads to Eq. (1) and the reported XMCD signals. It is an exact result, likewise our calculations leading to results in Eqs. (4) and (5) [16,18]. The Kramers doublet Eq. (3) is the outcome of a search for a minimal model that yields satisfactory paramagnetic and ordered magnetic moments Eq. (4), along with realistic XMCD signals in the ordered phase Eq. (5).

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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

The cubic structure of Ba₂NaOsO₆ at room temperature is defined by the space group Fm $\bar{3}$ m (No. 225), with a lattice parameter $\approx 8.281 \text{ \AA}$ (Table I in Ref. [9]). Tetragonal P4₂/mmn (No. 136, crystal class 4/mmm) with Os ions in Wyckoff position 2a (m.mm site symmetry) describes a paramagnetic phase [12]. Lattice vectors and origin of the subgroup in respect of the parent cubic structure are (1/2, -1/2, 0), (1/2, 1/2, 0), (0, 0, 1), and (0, 0, 0), respectively. The propagation vector for the symmetry lowering from cubic to tetragonal is $\mathbf{k} = (0, 0, 1)$. An electronic structure factor is taken to be [16],

$$\Psi_Q^K(\text{Pnn'm}') = \sum \exp(i\kappa \cdot \mathbf{d}) \langle \mathbf{T}_Q^K \rangle_{\mathbf{d}}, \quad (\text{A1})$$

where the sum is over the two positions $\mathbf{d}$ used by Os ions, and the reflection vector $\kappa = (h, k, l)$ with integer Miller indices h, k, l . The structure factor possesses information about the relevant Wyckoff positions available in the Bilbao table MWYCKPOS [13]. 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 [13]. Bulk properties studied in the main text are described by $\Psi_Q^K(\text{Pnn'm}')$ evaluated with $\kappa = 0$. Taken together, the two tables provide all information required to derive the final result Eq. (1).

A magnetic symmetry inferred from experimental results in Refs. [2,7,8,9] is a combination of two order parameters, an antiferrotype (AFM) associated with a propagation vector $\mathbf{k} = (0, 0, 1)$, and a ferrotype (FM) associated with $\mathbf{k} = (0, 0, 0)$. The two orders are depicted in Fig. 1, and their individual symmetries are [13]

(AFM) P₁nnm (No. 58.404), basis = {(0, 0, 1), (1/2, 1/2, 0), (-1/2, 1/2, 0)}, origin at (0, 0, 0), osmium ions in Wyckoff position 2a;
(FM) Im'm'm (No. 71.536), basis = {(0, 0, -1), (-1/2, 1/2, 0), (1/2, 1/2, 0)}, origin at (0, 0, 0), osmium ions in position 2a.

The presence of both order parameters implies that the magnetic symmetry of Ba₂NaOsO₆ is Pnn'm' (No. 58.398), with a basis $\xi = (1/2, 1/2, 0)$, $\eta = (-1/2, 1/2, 0)$, $\xi = (0, 0, 1)$, and origin (0, 0, 0). A spontaneous magnetization is permitted in the magnetic crystal class mm'm'. Osmium ions use position 2a in Pnn'm' with symmetry 2'/m'. Lattice parameters are $a = b \approx 5.856 \text{ \AA}$, $c \approx 8.281 \text{ \AA}$.

APPENDIX B

A matrix element in Eq. (2), for example, is calculated with [16,18,19]

$$\langle JM|T_Q^K|J'M'\rangle = (-1)^{J-M} \begin{pmatrix} J & K & J' \\ -M & Q & M' \end{pmatrix} (J||T^K||J'), \quad (\text{B1})$$

where the right-hand side includes a product of a 3j symbol (or a Clebsch-Gordan coefficient) and a reduced matrix element (RME) = $(J||T^K||J')$. RMEs are derived from Eq. (73) in Ref. [16], which is written in terms of a unit tensor for

several equivalent electrons using fractional parentage coefficients [18]. Notably, quantum numbers that define the core state in $(J||T^K||J')$ are gathered in one Racah 6j symbol (see Ref. [19] for analytic values of 6j symbols). Alternatively, for the simple case of one electron that is of immediate interest, Eq. (73) can be expressed in terms of a product of three Racah 6j symbols. Each symbol $\{ \}$ contains four triangle conditions [19]. Quantum numbers of the core state are spin $\sigma = 1/2$, total angular momentum Λ , and orbital angular momentum μ . For an E1-E1 event and a valence state orbital angular momentum l ,

$$(J||T^K||J') = -(-1)^{J'+\Lambda} (2\Lambda + 1) [(2J + 1)(2J' + 1)(2K + 1)]^{1/2} \left\{ \begin{matrix} J & \Lambda & 1 \\ \mu & l & \sigma \end{matrix} \right\} \left\{ \begin{matrix} J' & \Lambda & 1 \\ \mu & l & \sigma \end{matrix} \right\} \left\{ \begin{matrix} J' & \Lambda & 1 \\ 1 & K & J \end{matrix} \right\}. \quad (\text{B2})$$

Triangle conditions in Eq. (B2) include $\Lambda = \mu \pm \sigma$, $J = l \pm \sigma$, $J' = l \pm \sigma$, together with $J = |\Lambda - 1|$, Λ , $\Lambda + 1$, and likewise for J' . XMCD signals using an E1-E1 absorption event at L edges ($\mu = 1$, $l = 2$) depend on dipole matrix elements ($K = 1$), namely, $(3/2||T^1||3/2) = -(1/15)\sqrt{(2/15)}$, $(3/2||T^1||5/2) = -(5/2||T^1||3/2) = -(1/5)\sqrt{(3/10)}$ for the L_3 edge ($\Lambda = 3/2$), and $(3/2||T^1||3/2) = -(1/3)\sqrt{(5/6)}$ for the L_2 edge ($\Lambda = 1/2$). Expectation values of T^1 follow from Eq. (2), where the coefficients of f and f^* are, respectively,

$$\begin{aligned} \langle u|T_{+1}^1|\hat{u}\rangle &= \sqrt{(2/15)}(3/2||T^1||3/2)[1 + |t|^2]^{-1}, \\ \langle \hat{u}|T_{+1}^1|u\rangle &= -\sqrt{(2/5)}t(3/2||T^1||5/2)[1 + |t|^2]^{-1}. \end{aligned} \quad (\text{B3})$$

The expectation value of the magnetic moment follows from Eqs. (2) and (A3).

The coefficient of f in Eq. (2) is seen to be diagonal in J . For the magnetic moment it can be calculated with $(\mathbf{L} + 2\mathbf{S}) = g\mathbf{J}$ using an RME = $[J(J + 1)(2J + 1)]^{1/2}$ and a Landé factor $g = 4/5$ ($S = 1/2$, $L = 2$). Conversely, the coefficient of f^* in Eq. (2) is an off-diagonal matrix element, namely, that of $\mathbf{S}$ in $(\mathbf{L} + 2\mathbf{S}) = (\mathbf{J} + \mathbf{S})$ between states $J = 3/2$ and $5/2$. The required RME is obtained from Eq. (7.1.7) in Ref. [19].

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