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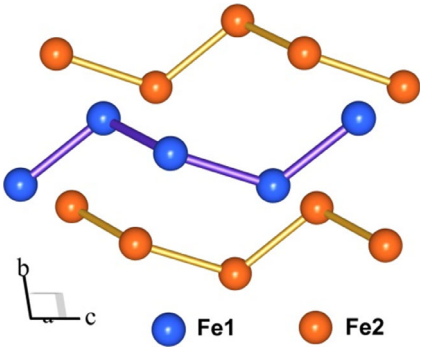
Self-Consistent Four-Particle Cluster Model of Fe^{3+} Heisenberg Chains: Spectral and Magnetic Properties of $YFe_3(BO_3)_4$ Crystals



A self-consistent four-particle cluster model of iron Heisenberg chains is developed. This model correctly accounts for the main physical features of 1D magnets. The model is tested by successfully simulating the optical spectra (measured in this work) and magnetic properties of a quasi-1D $YFe_3(BO_3)_4$, crystal containing helical chains of Fe^{3+} ions. It can be used to analyze the properties of multiferroic multifunctional rare-Earth iron borates.

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Self-Consistent Four-Particle Cluster Model of Fe^{3+} Heisenberg Chains: Spectral and Magnetic Properties of $YFe_3(BO_3)_4$ Crystals

Boris Z. Malkin, Elena A. Popova, Elena P. Chukalina, Artjoms Jablunovskis, and Marina N. Popova*

The magnetic properties of antiferromagnetic quasi-1D $YFe_3(BO_3)_4$ crystals are studied based on the analysis of the measured optical spectra of the Fe^{3+} ions in different rare-Earth (RE) iron borates and a self-consistent four-particle cluster approach to helical iron chains. The parameters of crystal fields affecting the Fe^{3+} ions are calculated in the framework of the exchange charge model. The parameters of the isotropic intrachain and interchain exchange interactions between the Fe^{3+} ions are determined from modeling the temperature dependences of magnetic susceptibilities, the phase transition temperature, and spontaneous magnetic moments. The magnetic easy-plane anisotropy is explained as the result of dipolar interactions between the Fe^{3+} ions in the trigonal crystal lattice. The developed model can be used to analyze and predict the properties of multiferroic multifunctional RE iron borates and highlight contributions of the iron subsystem into the magnetoelectric and magnetoelastic effects in these compounds.

Multiferroic rare-earth (RE) iron borates $REFe_3(BO_3)_4$ attract attention of researchers because of interesting magnetic, magnetoelectric, magnetoelastic,[1–3] magnetodielectric,[4] and optical properties,[5–8] some of which have an application potential. To completely realize this potential, it is necessary to build physically grounded models of different interactions in iron borates, which would allow one to correctly simulate magnetic, multiferroic, and optical properties of these compounds and develop the microscopic theory of the ME effect and other phenomena. The most significant structural feature of RE iron borates is the helical chains of FeO_6 octahedra.[6,9,10] This quasi-1D of the Fe magnetic subsystem is responsible, in particular, for relatively low Neel temperatures as compared with the energy of intrachain exchange interactions and for short-range correlations observed in RE iron borates at temperatures well above T_N.[11,12] In this Letter, we present a minimal model that quantitatively describes the physical properties of high-spin chains with different space structures (linear, zig-zag, or helical). The main idea is that using the exact diagonalization method and expanding the Bethe–Peierls approximation,[13] to clusters containing at least one internal pair of particles coupled with antiferromagnetic exchange interaction (i.e., at least two dimers), we can accurately take into account spin correlations of nearest neighbors. In particular, the essential drawbacks of previously used self-consistent single-site or dimer models in studies of RE iron borates, namely, a presence of a magnetic order in an isolated chain and strongly overestimated values of the exchange integrals and Neel temperatures,[14] are removed in the present work. To test the model, we choose the $YFe_3(BO_3)_4$ crystal containing only one magnetic system, namely, just the iron one.

$YFe_3(BO_3)_4$ crystals belong to the trigonal sp gr $P3_121$ at temperatures below 360 K.[10] The unit cell in the paramagnetic phase contains two types of structurally nonequivalent Fe^{3+} ions (Fe1 and Fe2 ions in the 3*a* and 6*c* positions, respectively, see **Figure 1**a), forming helical Fe1 and Fe2 chains along the *c*-axis. The lattice constants are $a = 0.95161$ nm and $c = 0.75441$ nm.[15] The Fe2 chains are shifted by ± 0.0088 nm along the *c*-axis from the *ab* planes containing the Fe1 and Y ions. Iron ions are sixfold coordinated by oxygen ions forming strongly deformed edge-sharing octahedra, the point symmetry groups are C_2 and C_1 at Fe1 and Fe2 sites, respectively. The R_{nn} distances between the nearest-neighbor iron ions in the chains are ≈ 0.315 nm; the next-nearest neighbors of Fe1 ions at a distance $R_{nnn} \approx 0.435$ nm are two Fe2 ions belonging to different Fe2 chains. The second neighbors of Fe2 ions are one Fe1 ion and one Fe2 ion.

Optical transitions of iron ions in $REFe_3(BO_3)_4$ lead to wide absorption bands which are practically independent of the

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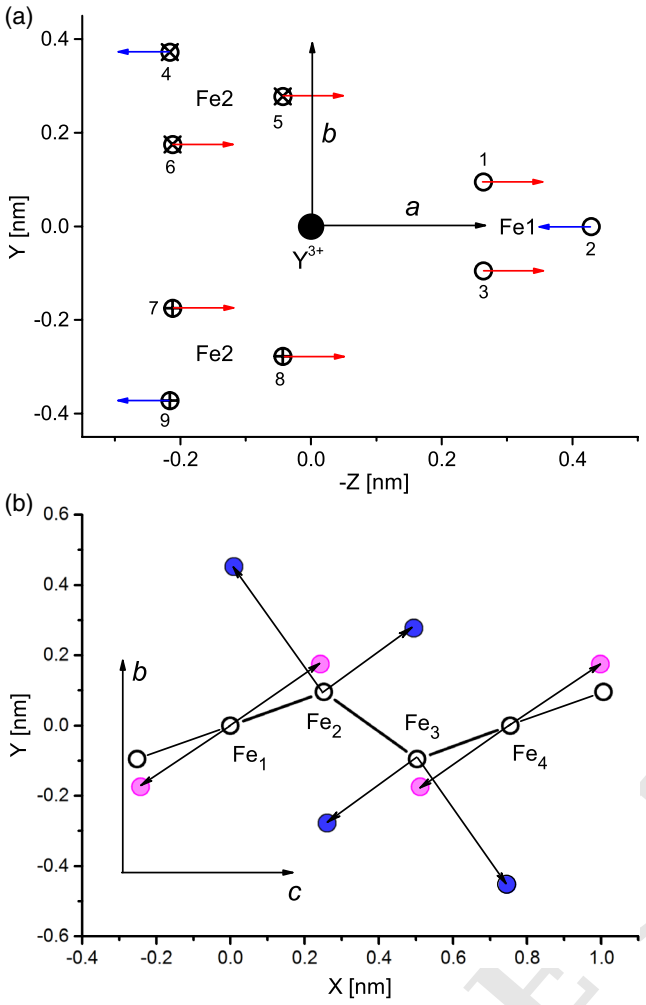

Figure 1. Projection of a) Fe1 (empty circles), Fe2 (circles with a cross), and yttrium (big black circle) ions in a unit cell of $YFe_3(BO_3)_4$ onto the *ab* plane. Magnetic moments at temperatures $T < T_N$ are shown by arrows. b) a Fe1 chain (empty circles) and the nearest-neighbor Fe2 ions (filled circles) from six different chains onto the *cb* plane. The global coordinate system is used with the axes $x \parallel c$, $y \parallel b$, $z \parallel -a$.

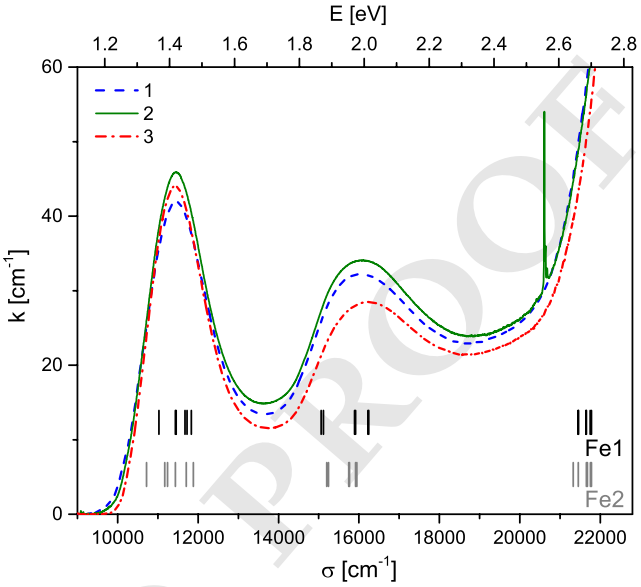

Figure 2. Absorption spectra of $YFe_3(BO_3)_4$ (1), $TbFe_3(BO_3)_4$ (2), and $GdFe_3(BO_3)_4$ (3) measured at 100 K and calculated wave numbers (sticks) of zero-phonon transitions in Fe^{3+} ions. A narrow line at about 20 600 cm^{-1} in 2 is due to transitions of the Tb^{3+} ions in $TbFe_3(BO_3)_4$.

specific RE ion (see **Figure 2**). Experimental details can be found in Supporting Information.

We use the measured spectra to verify the results (described in Supporting Information) of crystal-field (CF) calculations,[16,17] for the Fe1 and Fe2 ions, which are the first steps in developing a four-particle cluster model for the Fe^{3+} Heisenberg chain. Two independent sets of the calculated CF parameters for the Fe1 and Fe2 ions are given in Supporting Information (Table S1, Supporting Information). These CF parameters were used to calculate energies of states originating from the ground (^6S) and low-energy Fe^{3+} free-ion terms (^4G, ^4P, ^4D, ^2I), and they are listed in Supporting Information (Table S2, Supporting Information). Frequencies of spin-allowed ($\Delta S = 1$) zero-phonon radiative transitions of iron ions are shown by sticks in Figure 2. Having in mind possible Stokes shifts of electron-vibrational bands in the absorption spectra from zero-phonon lines to higher frequencies of up to 10^3 cm^{-1}, we argue that the results of calculations agree satisfactorily with the observed three broad bands in the measured spectra.

The ground state $^6S_{5/2}$ is split by CF and spin–orbit interactions into three Kramers doublets, but the total splitting is rather small, less than 2 cm^{-1}. For both the lowest doublets of the Fe1 and Fe2 ions, the *g* factor corresponding to the magnetic field direction along or close to the *c*-axis is about 10, but other two principal values of the *g* tensor are less than 0.2. Neglecting these small values, we get Ising-type doublets. The calculated magnetic susceptibilities of isolated Fe1 and Fe2 ions at temperatures below 5 K are strongly anisotropic (Figure S1, Supporting Information). However, as shown later, this single-ion easy-axis anisotropy, as well as the possible charge transfer effects,[18] is suppressed by strong isotropic exchange interactions.

The Hamiltonian of a cluster Fe_1—Fe_2—Fe_3—Fe_4 (see Figure 1b) in the space of 6^4 states corresponding to the ground multiplet $^6S_{5/2}$ of iron ions in the CF

$$H_{Cl} = H_{Cl}^{(0)} + H_{ex} + H_Z + H'_{ex} \quad (1)$$

includes the sum of energies of noninteracting ions $H_{Cl}^{(0)}$, exchange interactions inside the cluster $H_{ex} = -2J_1(\mathbf{S}_1\mathbf{S}_2 + \mathbf{S}_2\mathbf{S}_3 + \mathbf{S}_3\mathbf{S}_4)$, the Zeeman energy $H_Z = -(\mathbf{M}_1 + \mathbf{M}_2 + \mathbf{M}_3 + \mathbf{M}_4)\mathbf{B}$ in an external magnetic field **B**, and exchange interactions with the neighboring ions (with spin operators **S**') in the same chain and in six neighboring chains

$$H'_{ex} = -2J_1(\mathbf{S}_1\mathbf{S}'_1 + \mathbf{S}_4\mathbf{S}'_4) - 2J_2 \sum_{k=1,2,3,4} \mathbf{S}_k(\mathbf{S}'_{k,1} + \mathbf{S}'_{k,2}) \quad (2)$$

The matrices $\mathbf{M}_p$ and $\mathbf{S}_p$ represent the projections of operators of the magnetic and spin moments of the *p*-th iron ion onto the space of wave functions of the ground multiplet sublevels in

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the CF. To reduce the number of variable model parameters, we neglect possible differences in the exchange integrals in the Fe1 and Fe2 chains. Spin operators are related to magnetic moment operators by the relations $\mathbf{S}_p = \mathbf{g}_p^{-1}\mathbf{M}_p/\mu_B$ (μ_B is the Bohr magneton). Below, we neglect small differences (not exceeding 2×10^{-3}) between the calculated matrices $M_{p,\alpha}/\mu_B$ and $2S_{p,\alpha}$, $g_{p,\alpha\beta} = g\delta_{\alpha\beta}$ ($\alpha,\beta = x,y,z$), $g = 2$.

The effective Hamiltonian of a cluster in the paramagnetic phase can be written as

$$H_{\mathrm{Cl,eff}} = H_{\mathrm{Cl}}^{(0)} + H_{\mathrm{ex}} - (\mathbf{M}_1 + \mathbf{M}_4)\mathbf{B}_{\mathrm{loc}}^{(o)} - (\mathbf{M}_2 + \mathbf{M}_3)\mathbf{B}_{\mathrm{loc}}^{(i)} \quad (3)$$

where $\mathbf{B}_{\mathrm{loc}}^{(\lambda)}$ are magnetic fields affecting the pairs of inner ($\lambda = i$) and outer ($\lambda = o$) iron ions in the cluster, respectively. We determine the local susceptibilities $\kappa_{\alpha\beta}^{(\lambda\lambda)}$ of iron ions through the responses of their average magnetic moments to local fields $\mathbf{B}_{\mathrm{loc}}^{(\lambda)}$

$$<M_\alpha^{(\lambda)}> = \sum_{\beta\lambda'} \kappa_{\alpha\beta}^{(\lambda\lambda')} B_{\mathrm{loc},\beta}^{(\lambda')} \quad (4)$$

where $\mathbf{M}^{(i)}=(\mathbf{M}_2 + \mathbf{M}_3)/2$, $\mathbf{M}^{(o)}=(\mathbf{M}_1 + \mathbf{M}_4)/2$, and

$$\kappa_{\alpha\beta}^{(\lambda\lambda')} = \lim_{h\to 0} \mathrm{Tr}[M_\alpha^{(\lambda)}\rho(H_{\mathrm{Cl}}^{(0)} + H_{ex} - 2M_\beta^{(\lambda')}h)/h] \quad (5)$$

Here, $\rho(H)$ is the equilibrium density matrix of the system with the Hamiltonian H. The calculated local susceptibilities in the range of temperature $T > T_N = 38$ K are shown in Supporting Information (Figure S2, Supporting Information). The isotropic exchange interaction substantially suppresses the off-diagonal components of the single-ion susceptibility tensors (see Figure S1 and S2, Supporting Information), which we neglect below.

Furthermore, following the self-consistent field approximation, we replace operators of the spin and magnetic moments of iron ions surrounding the selected cluster by their average values. We obtain the following expressions for local fields where auxiliary magnetic fields $\Delta\mathbf{B}$(Fek) acting on the outer ions of a cluster are added,[13] ($J'_p = J_p/(g\mu_B)^2$, $p = 1, 2$)

$$\mathbf{B}_{\mathrm{loc}}^{(o)}(\mathrm{Fe1}) = \mathbf{B} + [2J'_1<\mathbf{M}(\mathrm{Fe1})> + 4J'_2<\mathbf{M}(\mathrm{Fe2})>] + \Delta\mathbf{B}(\mathrm{Fe1}) \quad (6)$$

$$\mathbf{B}_{\mathrm{loc}}^{(o)}(\mathrm{Fe2}) = \mathbf{B} + 2[J'_1<\mathbf{M}(\mathrm{Fe2})> + J'_2(<\mathbf{M}(\mathrm{Fe1})> + <\mathbf{M}(\mathrm{Fe2})>)] + \Delta\mathbf{B}(\mathrm{Fe2}) \quad (7)$$

$$\begin{aligned}\mathbf{B}_{\mathrm{loc}}^{(i)}(\mathrm{Fe1}) &= \mathbf{B} + 4J'_2<\mathbf{M}(\mathrm{Fe2})>,\\ \mathbf{B}_{\mathrm{loc}}^{(i)}(\mathrm{Fe2}) &= \mathbf{B} + 2J'_2[<\mathbf{M}(\mathrm{Fe1})> + <\mathbf{M}(\mathrm{Fe2})>]\\ \mathbf{B}_{\mathrm{loc}}^{(i)}(\mathrm{Fe2}) &= \mathbf{B} + 2J'_2[<\mathbf{M}(\mathrm{Fe1})> + <\mathbf{M}(\mathrm{Fe2})>]\end{aligned} \quad (8)$$

These fields are determined from the condition imposed on the average magnetic moments

$$<\mathbf{M}^{(o)}> = <\mathbf{M}^{(i)}> = <\mathbf{M}(\mathrm{Fe}k)> = \chi(\mathrm{Fe}k)\mathbf{B} \quad (9)$$

where χ(Fek) is the magnetic susceptibility of the ions Fek ($k = 1, 2$). Substituting Equation (6)–(8) into Equation (4), we obtain a coupled system of equations for $<\mathbf{M}$ (Fek)>

$$<\mathbf{M}(\mathrm{Fe1})> = \chi_0(\mathrm{Fe1})[\mathbf{B} + 4J'_2<\mathbf{M}(\mathrm{Fe2})>] \quad (10)$$

$$<\mathbf{M}(\mathrm{Fe2})> = \chi_0(\mathrm{Fe2})[\mathbf{B} + 2J'_2(<\mathbf{M}(\mathrm{Fe1})> + <\mathbf{M}(\mathrm{Fe2})>)] \quad (11)$$

where $\chi_0(\mathrm{Fe}k) = (\kappa^{(ii)}\kappa^{(oo)} - \kappa^{(io)2})/(\kappa^{(oo)} - \kappa^{(io)})$. Its solution gives the susceptibilities χ(Fek) (see Equation S2–S4, Supporting Information). From a comparison of the calculated susceptibilities $\chi = \chi(\mathrm{Fe1}) + 2\chi(\mathrm{Fe2})$ with the measurement data[19] ($\chi_{||} = \chi_{cc}$, $\chi_\perp = (\chi_{aa} + \chi_{bb})/2$), we obtained the exchange integrals $J_1 = -5.5$ K and $J_2 = -3.45$ K. It should be noted that neglecting the quantum fluctuations of the magnetic moments (replacing the spin operators by their average values) leads to significantly higher values of the exchange integrals compared with actual values to reproduce the measured susceptibility. The matter is that the increased antiferromagnetic exchange interaction compensates for the reduction in the magnetic moment due to fluctuations.

In the antiferromagnetic phase, the magnetic moments of neighboring ions in helical chains are antiparallel, $\mathbf{M}_1 = -\mathbf{M}_2 = \mathbf{M}_3 = -\mathbf{M}_4$. As follows from the measurement data,[20] and the results of the calculation of magnetic anisotropy (see below), the magnetic moments of iron ions in the antiferromagnetic phase are perpendicular to the c-axis. The most natural assumption is that they are aligned along one of the three C_2 axes. (The problem of calculating the sixth-order anisotropy constant, which is determined in the case of a trigonal system by magnetoelastic interaction, is beyond the scope of this Letter.) At the phase-transition temperature T_N, the response of the system to a spatially inhomogeneous magnetic field (staggered field $\mathbf{B}_s$), the direction of which at the positions of the iron ions coincides with the directions of their magnetic moments, diverges. The calculation of this response, i.e., of the antiferromagnetic susceptibility, is carried out similarly to the above derivation of the expression for paramagnetic susceptibility by considering a four-particle cluster in a chain subjected to a staggered field $\mathbf{B}_s$ (for details, see Supporting Information). The antiferromagnetic susceptibilities of the subsystems of ions Fe1 and Fe2 are obtained in the form

$$\chi_s(\mathrm{Fe}k) = \chi_{0s}(\mathrm{Fe}k)\{1 + 2J'_{2R}[\chi_{0s}(\mathrm{Fe1}) + \chi_{0s}(\mathrm{Fe2}) - \chi_{0s}(\mathrm{Fe}k)]\}/\Delta_s \quad (12)$$

Here, $\Delta_s = 1 + 2J'_{2R}\chi_{0s}(\mathrm{Fe2}) - 8J'^2_{2R}\chi_{0s}(\mathrm{Fe1})\chi_{0s}(\mathrm{Fe2})$ and $\chi_{0s} = (\kappa_s^{(ii)}\kappa_s^{(oo)} - \kappa_s^{(io)2})/(\kappa_s^{(oo)} - \kappa_s^{(io)})$, where $\kappa_s^{(\lambda\lambda')}$ are local susceptibilities defined by Equation (5) for the corresponding chains in the staggered field $\mathbf{B}_s$. Note that, when considering the intercluster interactions in the antiferromagnetic phase, we introduce renormalized exchange integrals $J_{pR} = R_p J_p$ ($p = 1,2$), where R_p is the reduction factor. The expression for the denominator Δ_s in Equation (12) demonstrates the formation of a long-range order, explicitly, due to the exchange interchain interaction (with the exchange integral J_{2R}) and, indirectly, due to exchange interactions in the chains which determine the temperature dependence of the susceptibilities of isolated clusters $\chi_{0,s}$(Fek). The transition temperature satisfies the equation

$$\chi_s(T_N)^{-1} = [\chi_s(\mathrm{Fe1}, T_N) + 2\chi_s(\mathrm{Fe2}, T_N)]^{-1} = 0 \quad (13)$$

Additional restrictions on the magnitude of the exchange integrals J_{pR} are obtained from the consideration of the spontaneous

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magnetic moments of iron ions. The spontaneous moments are determined by the system of coupled self-consistent equations

$$M_s(\mathrm{Fe}k) = \langle M_{1a}\rangle = \langle M_{3a}\rangle = -\langle M_{2a}\rangle = -\langle M_{4a}\rangle = \mathrm{Tr}[M_{1a}\rho(H_{\mathrm{Cl,af}}(\mathrm{Fe}k))] \quad (14)$$

where $H_{\mathrm{Cl,af}}(\mathrm{Fe}k)$ is the effective cluster Hamiltonian in the antiferromagnetic phase in zero external field. The temperature dependence of the average magnetic moment $M = [M_s(\mathrm{Fe1}) + 2M_s(\mathrm{Fe2})]/3$ calculated in accordance with Equation (14) at the reduction coefficients $R_1 = 0.463$ and $R_2 = 0.264$ agrees satisfactorily with the data of neutron diffraction measurements[20] (see Figure S3, Supporting Information). When used in the calculations, the reduction factors presented earlier, the solution $T_N = 38$ K of Equation (13) coincides with the measurement data (see Supporting Information and Figure S5 therein).

In the case of S-state ions, magnetic dipolar interactions play a dominant role in the formation of magnetic anisotropy. We considered the contribution of the dipolar interactions to the energy of the iron subsystem in $YFe_3(BO_3)_4$ as a function of an angle θ between the *c*-axis and the iron magnetic moments $\mathbf{M}_{\mathrm{Fe}k}$, assuming a collinear antiferromagnetic structure formed by the parallel magnetic moments of ions lying in (Fe1 ions in the sublattice 2 with moments $\mathbf{M}_{\mathrm{Fe1}}$) or close to (Fe2 ions with moments $\mathbf{M}_{\mathrm{Fe2}}$ in sublattices 4 and 9, see Figure 1a) a fixed *ab* plane and antiparallel to moments of ions in neighboring *ab* planes shifted along the *c*-axis by $\pm c/3$ (sublattices 1, 6, 8 and 3, 5, 7). The sums over the crystal lattice with the unit cell of $YFe_3(BO_3)_4$ doubled along the *c*-axis were calculated using the Ewald method. The obtained energy of the magnetic subsystem in the assumed antiferromagnetic structure with $\mathbf{M}_{\mathrm{Fe}k} = \mathbf{M}$ equals

$$E = [2(J_{1R} + J_{2R})/\mu_B^2] - \frac{138.1\pi}{27v}(1 - 3\cos^2\theta)]M^2 \quad (15)$$

where $v = \sqrt{3}a^2c$ is the unit-cell volume. Substituting the numerical values of the parametersinto Equation (15), we obtain $E = [-8.29 - 0.0085(1 - 3\cos^2\theta)](M/\mu_B)^2$ in degrees Kelvin. As shown, the energy of magnetic anisotropy is three orders of magnitude lower than the energy of exchange interactions. Dipole–dipole interactions practically do not affect the temperature of phase transition, but they determine the easy-plane type of the magnetic structure. The energy of the magnetic subsystem is minimal when the magnetic moments are oriented in a plane perpendicular to the *c*-axis. An estimate of the magnetic anisotropy field H_A parallel to the *c*-axis, in which the Zeeman energy compensates for the increase in the energy of iron ions when the magnetic moment $M \approx 4\,\mu_B$ rotates from the plane to the *c*-axis, yields $H_A = 1.51$ kOe, which is close to that found from the measurements of the antiferromagnetic resonance spectra at $T = 4.2$ K (1.44 kOe).[21]

In the magnetically ordered phase, induced by an external magnetic field, changes of magnetic moments of inner and outer iron ions in a cluster can be written similarly to Equation (4) with the local susceptibilities defined by the expression

$$\kappa_{\alpha\beta}^{(\lambda\lambda')} = \lim_{h\to 0}\mathrm{Tr}\{M_\alpha^{(\lambda)}[\rho(H_{\mathrm{Cl,af}} - 2M_\beta^{(\lambda')}h) - \rho(H_{\mathrm{Cl,af}})]/h\} \quad (16)$$

The local magnetic fields can be written similarly to Equation (6)–(8) where it is enough to replace J_1, J_2 and $\mathbf{M}(\mathrm{Fe}k)$ by J_{1R}, J_{2R}, and $\Delta\mathbf{M}(\mathrm{Fe}k)$, respectively. The auxiliary fields $\Delta\mathbf{B}(\mathrm{Fe}k)$ and the effective single-ion susceptibilities $\chi(\mathrm{Fe}k)$ are determined by the condition of equivalence of iron ions with different directions of spontaneous moments in weak external fields: $\langle\Delta\mathbf{M}^{(o)}\rangle = \langle\Delta\mathbf{M}^{(i)}\rangle = \langle\Delta\mathbf{M}(\mathrm{Fe}k)\rangle = \chi(\mathrm{Fe}k)\mathbf{B}$. The temperature dependences of the local susceptibilities $\kappa_{\alpha\beta}^{(\lambda\lambda')}$ at temperatures $T < T_N$ are shown in Figure S2, Supporting Information. The antiferromagnetic exchange interaction suppresses single-ion magnetic anisotropy, the off-diagonal components of the susceptibility tensor take values smaller than the diagonal components by three orders of magnitude.

The calculation results on the components of the magnetic susceptibility tensor of a $YFe_3(BO_3)_4$ crystal in the paramagnetic and antiferromagnetic phases are compared with the measurement data[19] in **Figure 3**. The susceptibility in the antiferromagnetic phase in magnetic fields perpendicular to the *c*-axis, $\chi_\perp = (\chi_{aa} + \chi_{bb})/2$, is obtained by averaging over three possible domains with orientations of magnetic moments along the three C_2 axes. Figure 3 shows a good agreement between the calculated and measured susceptibilities in boththe paramagnetic and antiferromagnetic phases. In particular, the nonmonotonous behavior of the low-temperature ($T < T_N$) susceptibility, $\chi_\parallel = \chi_{cc}$, which was also observed for the easy-plane antiferromagnets $EuFe_3(BO_3)_4$ and $SmFe_3(BO_3)_4$,[1] with the dominant contributions of the iron subsystem to susceptibility, is reproduced by the presented model.

A model of four-particle self-consistent clusters in helical iron chains is developed, which can be used for the physically grounded modeling of various properties of functional RE iron borates, taking into account the quasi-1D of the iron subsystem. This model was tested by simulating the properties of $YFe_3(BO_3)_4$ crystals containing only the iron magnetic system. The parameters of CFs acting on the Fe^{3+} ions and the energy spectra of the $3d^5$ electronic shell of Fe^{3+} in $YFe_3(BO_3)_4$ were calculated. The obtained frequencies of spin-allowed zero-phonon

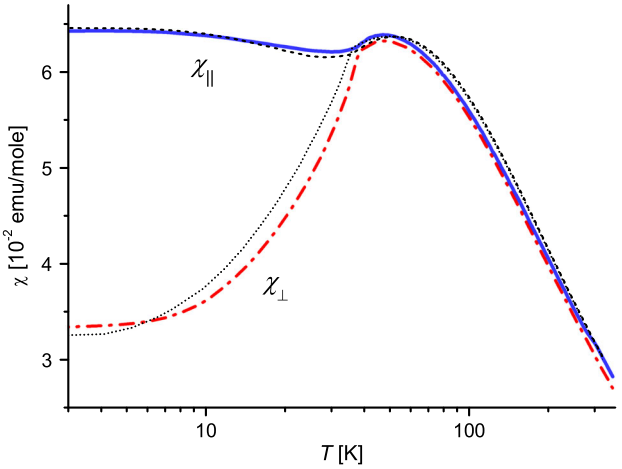

Figure 3. Temperature dependences of the components of the magnetic susceptibility tensor for $YFe_3(BO_3)_4$. Black dotted lines are the results of calculations, blue solid and red dash-dotted lines are the measurement data.[19]

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radiative transitions in iron ions correlate satisfactorily with the measured absorption spectra of different RE iron borates. Then, presented earlier in the literature, temperature dependences of components of the magnetic susceptibility tensor of $YFe_3(BO_3)_4$ in both the paramagnetic and antiferromagnetic phases were successfully simulated using the developed four-particle cluster model. A good agreement between the experimental and calculated data testifies a good quality of the model. The model can be used to analyze properties of the entire family of multifunctional RE iron borates and highlight the contribution of the iron subsystem into these properties.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

crystal fields, Fe chains, four-particle clusters, magnetic anisotropies, magnetic susceptibilities, optical spectra, $YFe_3(BO_3)_4$

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