Single ionic properties of $R_2Fe_{14}B$, RRu_2Si_2 and RNi_5 (R: rare earth element) calculated with ATOMIC MATTERS and ATOMIC MFA computation systems

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Abstract

The single ionic properties of paramagnetic ions are the core magnetic properties of magnetic materials. We present examples of calculation results for compounds $RE_2Fe_{14}B$, $RERu_2Si_2$ and $RENi_5$ (RE: rare earth element), generated with our computation systems ATOMIC MATTERS and ATOMIC MFA. The synergy of the ATOMIC MATTERS and ATOMIC MFA systems makes it possible to describe magnetic, calorimetric, and spectroscopic properties of atomic-like localized electron systems that are subject to electrostatic interactions taken as Crystal Electric Field (CEF), spin-orbit coupling, and magnetic interactions, taken as both Mean Field Approximation (MFA) and external magnetic fields. Our solution applies to situations in which any unclosed electron subshell of an ion interacts with the electrostatic potential of definable symmetry and the magnetic field comes from induced moments of identical paramagnetic neighbors. In this paper, we present some 4f (rare earth) cases of hard magnetic materials. Based on CEF and MFA theoretical methods, we are able to analyze the magnetization process and magnetic phase transition of materials as a function of temperature and an external magnetic field. These calculation systems make it possible to predict macroscopic properties such as magnetic moment (spin, orbit and total, and its directional components), localized electron specific heat c_{mol} (both Schottky-like type and λ-type), magnetic entropy, magneto-crystalline anisotropy constants $K_i(T)$, energy levels and total free energy as temperature dependences in a definable region of temperature, including the phase-transition region.

We emphasize the importance of symmetry of charge surroundings of an atom/ion, spin-orbit interactions (spin-orbit coupling) and the use of complex number matrices in the definition of the Hamiltonian.

Our computation systems make it possible to understand existing materials and are useful for developing new materials for permanent magnet technology.

1. Introduction

Materials with special magnetic properties are of great importance. The ability to perform fine electronic structure calculations of paramagnetic ions became the motivation to create software that can predict the properties of solid compounds with localized electron states and to help create new materials with properties dedicated to specific applications. Our aim was to find and parameterize the most important interactions in atoms and ions in ligand environments. Such parameterization, which comes directly from Crystal Electric Field (CEF) theory, makes it possible to transfer the influence of local charge surroundings between different ions. We decided to call our computation system ATOMIC MATTERS. Algorithms and technical details of ATOMIC MATTERS computation system are published at [1] and are available on the software web page [2], together with hundreds examples of calculations of ions of selected materials from different areas of the periodic table.

Single atomic properties calculated by ATOMIC MATTERS accurately describe properties of materials in defined temperature regions. We have calculated properties of materials in both paramagnetic and ordered states for over 100 real materials [2]. Although the static ATOMIC MATTERS calculations are surprisingly useful, they cannot provide descriptions of phase transitions. Therefore, we decided to create an extension for ATOMIC MATTERS software for phase-transition simulations according the Mean Field Approximation model. We present the concept and

scientific methods our computation systems called ATOMIC MATTERS and ATOMIC MATERS MFA.

This is the first presentation of the new computer package ATOMIC MATERS MFA that can describe the physical properties of atomic localized electron systems in self-organizing magnetic surroundings of identical ions/atoms. ATOMIC MATTERS MFA can simulate phase transitions of ionic/atomic systems according to dynamic calculations of the molecular field B_{mol}, simply defined as:

$$\mathbf{B}_{mol}(T) = n_{mol}\mathbf{m}(T)$$

that interacts with ions to induct their magnetic moment. Such self-agreed calculations can be performed after establishing only the molecular field factor n_{mol} that is closely related to the temperature of phase transitions (T_C or T_N). Our solution applies to situations in which an unclosed electron 3d/4d/5d/4f/5f subshell interacts with the electrostatic potential of definable symmetry (taken as a CEF) and the external magnetic field of identical neighbors.

2. Main assumptions of the theoretical approach

ATOMIC MATTERS and ATOMIC MATTERS MFA Computation Systems provide calculation methods under the following scientific assumptions:

• All 3d/4d/5d/4f/5f ions have a structure of discrete electron states that affects the properties of the whole compound.
• A description of multi-electron 3d^n, 4d^n, 5d^n, 4f^n, 5f^n systems is based on atomic physics, with atomic numbers S, L of the entire shell. This results in a space of n=(2S+1)(2L+1) states.
• In a solid, an atom/ion interacts with the electric potential (Stark effect) of the charge environment. This interaction leads to a reduction of the degeneracy of states and is referred to as the CEF (Crystal Electric Field).
• Through modifications of the fine structure of electron states of an atom/ion, CEF determines its properties in a crystal lattice, which corresponds to the properties of the whole crystal.
• Spin-orbit coupling makes an important contribution to the structure of states and must be taken into account in the calculations.
• Magnetic interactions, both inter-ionic exchange interactions and with the external field, lead to further

reduction of state degeneracy (Zeeman effect).
• The magnetic ordering is reflected in the symmetry breaking of the eigenfunctions of many-electron states.

We emphasize the fundamental role of the local symmetry of the environment of the paramagnetic ion in the crystal, taken into account using Crystal Electric Field (CEF) and spin-orbit formalism.

As a consequence of our assumptions, the electronic system is described according to atomic physics, by quantum numbers S, L (and J when it a good quantum number) of the whole shell. The ground term/multiplet is determined by Hund's rules. Then we work in the space of (2S+1)(2L+1) states. The calculated eigenvectors and expected values define spin and orbital magnetic moments of whole ions in both paramagnetic and ordered states.

In a solid, the open shell atom undergoes charge interactions from the surrounding charge distribution [3,4]. These interactions are known as crystal-field (CEF, CF) or sometimes zero field splitting (ZFS). Crystal-field interactions result in the fine (discrete) electronic structure of an atom in a solid that largely determines the properties of the whole compound in a solid state. This fine electronic structure is very sensitive to local symmetry. The symmetry of the local surrounding is reflected in the symmetry of the crystal-field (CEF) Hamiltonian.

3. Theoretical methods

Our theoretical approach is deeply rooted in atomic physics. Individual population of states of the fine electronic structure of ions/atoms are taken into account Boltzmann statistics and defining the temperature dependence of properties such as:

• full structure of discrete electron levels E_i (or E_i (T) for the magnetization process (ATOMIC MATTERS MFA only) in chosen calculation space $|J,J_z>$ or $|L,S,L_z,S_z>$ space
• Helmholtz free energy F(T)
• internal energy U(T)
• magnetic entropy $S_{mag}(T)$
• magnetic susceptibility calculated for different directions of external field $\chi^i(T)$ in a paramagnetic temperature region

- formation of magnetic ordered state (ATOMIC MATTERS MFA only)
- localized electronic contribution to specific heat $c_{Schottky}(T)$ for stable energy levels for structure E_i and for magnetic phase transitions (ATOMIC MATTERS MFA -only)
- probability of transitions (excitations) between eigenstates and spectra simulations including INS (Inelastic Neutron Scattering)
- magnetic moment and magnetization in ordered state (ATOMIC MATTERS MFA only)
- spin and orbital contribution to angular momentum of the entire electron subshell;
- magnetocrystalline anisotropy constants $K_i(T)$ (ATOMIC MATTERS MFA only);

For calculations in the thermodynamically stable temperature region, ATOMIC MATTERS offers the following CEF+Spin-Orbit+Zeeman Hamiltonian:

$$H_J = H_{CEF} + H_{Zeeman} = \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(J,J_z) + g_L \, \mu_B \, \mathbf{J} \cdot \mathbf{B}_{ext}$$

or

$$H_{LS} = H_{CEF} + H_{S-O} + H_{Zeeman} =$$
$$= \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(L,L_z) + \lambda \mathbf{L} \cdot \mathbf{S} + \mu_B (\mathbf{L} + g_e \, \mathbf{S}) \cdot \mathbf{B}_{ext}$$

according to the chosen calculation space of ground multiplet $|J,J_z\rangle$ [3-9] or the ground atomic term $|L,S,L_z,S_z,\rangle$ [10] respectively. For all Hamiltonians, B_n^m denotes CEF parameters, $\mathbf{O}_n^m$ are Stevens operators, λ is the spin–orbit constant, g_L, $g_e \approx 2.002324$ are the gyromagnetic factors. For a whole ion and electron respectively, μ_B is the Bohr magneton:

$$\mu_B = \frac{e\hbar}{2m_e}$$

and $\mathbf{B}_{ext}$ is the external magnetic field.

In all cases, calculations in the $|L,S,L_z,S_z,\rangle$ space are more physically appropriate due to their completeness, but traditional calculations with base $|J,J_z\rangle$ can be performed by our computation systems for comparisons and quick estimations [12].

For calculating properties at temperatures around the magnetic phase transition point, we use self-consistent methodology for molecular field calculation called Mean Field Approximations. The idea behind this

method is the estimation of the direction and value of the magnetic field (molecular field) generated by ions at a defined temperature, and calculating the influence of this magnetic field on the structure of the electronic states of an ion. According to the chosen calculation space, we define the molecular field as:

$$\mathbf{B}_{mol} = -n_{mol}\, g_L \mu_B < \mathbf{J} > \quad \text{or}$$

$$\mathbf{B}_{mol} = -n_{mol}\, \mu_B < \mathbf{L} + g_e \mathbf{S} >$$

so, the molecular field Hamiltonian has the form [10]:

$$H_{mol} = -n_{mol}\, g_L^2 \, \mu_B^2 \left(\mathbf{J} < \mathbf{J} > -\frac{1}{2} < \mathbf{J} >^2 \right)$$

or

$$H_{mol} = -n_{mol}\, g_L^2 \, \mu_B^2 \left((\mathbf{L} + g_e \mathbf{S}) < \mathbf{L} + g_e \mathbf{S} > -\frac{1}{2} < \mathbf{L} + g_e \mathbf{S} >^2 \right)$$

Because of the calculated electronic structure E_i, the directional components of magnetic moments will be established for all identical ions. This means that Hamiltonian matrix diagonalization is done for all defined temperature steps recurrently, contrary to simple ATOMIC MATTERS calculations which diagonalize matrix once for a single run. This self-consistent procedure has one only free parameter: n_{mol}, called the molecular field parameter. The value of n_{mol} is closely related to the temperature of phase transition T_N or T_C of the macroscopic structure of ions. The formal expression of the full Hamiltonian used by ATOMIC MATTERS MFA computation system has the form:

$$H_{J\,mol} = H_J + H_{mol} = +\sum_n \sum_m B_n^m \, \hat{\mathbf{O}}_n^m(J,J_z) +$$
$$+ n_{mol}\, g_L^2 \, \mu_B^2 \left(-\mathbf{J} < \mathbf{J} > +\frac{1}{2} < \mathbf{J} >^2 \right) + g_L \, \mu_B \, \mathbf{J} \cdot \mathbf{B}_{ext}$$

or

$$H_{LS\,mol} = \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(L,L_z) + \lambda \mathbf{L} \cdot \mathbf{S} +$$
$$+ n_{mol}\, \mu_B^2 \left(-(\mathbf{L} + g_e \mathbf{S}) < \mathbf{L} + g_e \mathbf{S} > +\frac{1}{2} < \mathbf{L} + g_e \mathbf{S} >^2 \right)$$
$$+ \mu_B (\mathbf{L} + g_e \mathbf{S}) \cdot \mathbf{B}_{ext}$$

according to the chosen calculation space $|J,J_z\rangle$ or $|L,S,L_z,S_z,\rangle$ respectively.

The eigenvectors of the Hamiltonian are described according to the selected base of calculations by the total momentum quantum numbers $|J,J_z\rangle$ or spin and orbit quantum numbers $|L,S,L_z,S_z,\rangle$.

Using the commutation relations of the angular momentum operators, we obtain information about the expected values of the projections of magnetic momentum of all electronic states at a specified temperature [3]-[6], [9].

$$m_J^\alpha(T) = \frac{g_L\mu_B}{Z(T)}\sum_i <J_\alpha^i> \exp\left(-\frac{E_i(T)}{k_B T}\right)$$

$$m_{LS}^\alpha(T) = \frac{\mu_B}{Z(T)}\sum_i <L_\alpha^i + g_e S_\alpha^i> \exp\left(-\frac{E_i(T)}{k_B T}\right)$$

where α indexes directional components, i - numbers the Hamiltonian eigenstates, while $<J_\alpha>$ represents the expected value of the total angular momentum along the α-axis in the i-th state.

All property calculations can be done for 3D (x,y,z) real space using complex Hamiltonian matrix elements defined by full expressions of Stevens O^n_m operators. Mostly for comparison with traditional calculation results, ATOMIC MATTERS computation systems also offers, 2D (x,z) calculation methodology of a simplified model of CEF interactions defined by Stevens O^n_m operators with real number matrix elements only [].

Taking into consideration the possibility of the thermal population of states, we automatically obtain thermal evolution of the single ion properties of a whole compound. This technique is based on the equivalent operator theory [4], defined as the CEF broadened by thermodynamic and analytical calculations, defined as the supplement of the CEF theory by including thermodynamic and analytical calculations.

At a temperature of T = 0 K, only the ground state is occupied. In this situation, the magnetic moment of the ion is exactly equal to the momentum of the ground state. At extremely low temperatures, it is possible to excite the system e.g. by magnetic interaction with low-energy neutrons (as is used in Inelastic Neutron Scattering Spectroscopy, INS). Spectra simulations for this situation and for the different thermal limitations of

the population of excited states and methodological limitations are provided by ATOMIC MATTERS computation system.

When the temperature rises, the probability of higher states being occupied increases according to Boltzmann statistics [11]. The number of ions with energy E_i within a system at a given temperature is:

$$N_i(T) = N_0 \frac{\exp\left(-\frac{E_i(T)}{k_B T}\right)}{Z(T)};$$

In the above expression, N denotes the total number of particles and Z(T) is the statistical sum of states (partition function). The most sensible value is $N=N_0\approx6.022.10^{23}$ mol^{-1} (Avogadro constant). Knowing the statistical sum of the states, we can determine the Helmholtz free energy F(T):

$$F(T) = -k_B T \ln Z(T)$$

Which makes it possible to estimate the internal energy U(T) of the system:

$$U(T) = F(T) - T\left(\frac{\partial F(T)}{\partial T}\right) = -k_B T \frac{\partial}{\partial T}\left(\frac{F(T)}{k_B T}\right)$$

According to thermodynamic principles, in case of temperature stable energy states $E_i(T)$=const, the localized electrons' contribution to total specific heat of a material has the Schottky formula:

$$c_{Schottky}(T) = \left(\frac{\partial U(T)}{\partial T}\right)_{E_i}$$

In general, especially for temperature regions around transition temperature T_C or T_N, we calculate localized electron specific heat directly by numerical differentiation from Helmholtz free energy:

$$c_{mol}(T) = -T\left(\frac{\partial^2 F(T)}{\partial T^2}\right)$$

The fine structure of states (E_i, Γ_i) makes it possible to determine the thermodynamic functions for the statistical group of N_0=6.022.10^{23} mol^{-1} (Avogadro constant) ions. Taking into account the relationship between the thermodynamic functions, magnetic susceptibility within the limit of low external fields is defined as the product of:

$$\chi^{\alpha}(T) = \frac{\partial M_{\alpha}(T)}{\partial B_{\alpha}} = \frac{k_B T}{B_{\alpha}}\left(\frac{\partial \ln Z(T)}{\partial B_{\alpha}}\right)$$

Where α-index denotes Cartesian coordinates related to axes in the crystal lattice.

In our methodology, calculating magnetization amounts to summing the identically behaving magnetic moments of individual ions with an unclosed electron shell. Due to the fact that open subshell ions are in a self-aligned molecular field, their magnetic moment changes with temperature. Bearing in mind that each eigenstate of the CEF Hamiltonian is related to its magnetic moment, the total moment of a strongly correlated electron system at a given temperature is the resultant moment of occupied states calculated with the inclusion of the Boltzmann weight:

$$M_{\alpha}(T) = k_B T\left(\frac{\partial \ln Z(T)}{\partial B_{\alpha}}\right) = g_L \mu_B \sum_i N_i(T) < \Gamma_i(T)| \mathbf{J}_{\alpha} |\Gamma_i(T)>$$

$$M_{\alpha}(T) = k_B T\left(\frac{\partial \ln Z(T)}{\partial B_{\alpha}}\right) =$$
$$= \mu_B \sum_i N_i(T) < \Gamma_i(T)| (\mathbf{L}_{\alpha} + g_e\mathbf{S}_{\alpha}) |\Gamma_i(T)>$$

where α indexes directional components, i numbers the Hamiltonian eigenstates, while $<\mathbf{J}_{\alpha}>$ represents the expected value of the total angular momentum operator. This approach provides a clear way to determine the components of the total magnetic moment of paramagnetic ions.

ATOMIC MATTERS MFA provides single-ionic magnetocrystalline anisotropy calculations include full calculations (without Brilluin functions approximation) of magnetocrystalline constants $K_i(T)$ for defined range of temperature according to relations [12]:

$$K_1(T) = \frac{3}{2}B_2^0\left(\langle\hat{\mathbf{O}}_2^0\rangle - \langle\hat{\mathbf{O}}_2^2\rangle\right) - 5B_4^0\left(\langle\hat{\mathbf{O}}_4^0\rangle - 3\langle\hat{\mathbf{O}}_4^2\rangle\right) -$$
$$- \frac{21}{2}B_6^0\left(\langle\hat{\mathbf{O}}_6^0\rangle - 5\langle\hat{\mathbf{O}}_6^2\rangle\right),$$

$$K_2(T) = \frac{35}{8}B_4^0\left(\langle\hat{\mathbf{O}}_4^0\rangle - 4\langle\hat{\mathbf{O}}_4^2\rangle + \langle\hat{\mathbf{O}}_4^4\rangle\right) +$$
$$+ \frac{63}{8}B_6^0\left(\langle\hat{\mathbf{O}}_6^0\rangle - 20\langle\hat{\mathbf{O}}_6^2\rangle + 5\langle\hat{\mathbf{O}}_6^4\rangle\right),$$

$$K_2^*(T) = \frac{1}{8}\left(B_4^0\langle\hat{\mathbf{O}}_4^0\rangle + 5B_6^4\langle\hat{\mathbf{O}}_6^4\rangle\right),$$

$$K_3(T) = -\frac{231}{16}B_6^0\langle\hat{\mathbf{O}}_6^0\rangle, \quad K_3^*(T) = -\frac{11}{16}B_6^4\langle\hat{\mathbf{O}}_6^4\rangle.$$

Where: $\langle\hat{\mathbf{O}}_n^m\rangle$ denotes of thermal expected values o Stevens operators.

4. Calculation results

According to described methodology, we present the calculations results for some well-known magnetic compounds from isostructural series: RRu_2Si_2, RNi_5 and $R_2Fe_{14}B$ (R: rare earth element). We do not look for new sets of CEF parameters for these compounds and molecular field parameter either. This is the premiere presentation of our software, so we would like to show the results of calculations performed by our computation systems under established parameters taken from literature for the ATOMIC MATTERS MFA calculation methodology and effectiveness evaluation. This will clearly express the differences between simplified, older calculations of various researchers and the methodology of ATOMIC MATTERS MFA computation systems.

3.1. Results for RNi_5 family of compounds

a. Results of calculations of Nd^{3+} ions on $NdNi_5$ solid compound according to parameters: B_2^0=3.35K, B_4^0=14.5mK, B_6^0=-0.35mK, B_6^6=-13.5mK. Taken from: [13], [15]

c. Results of calculations of Er^{3+} ions on $ErNi_5$ solid compound according to parameters: B_2^0=-0.615K, B_4^0=-2.5mK, B_6^0=23.2μK, B_6^6=0.132mK. Taken from: [15]
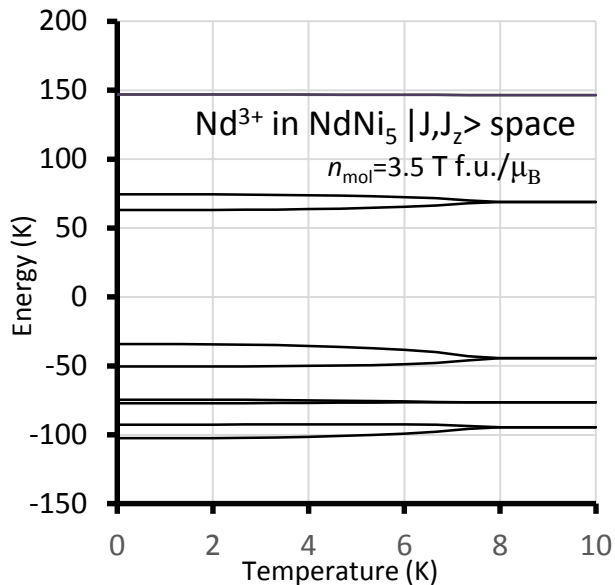
Fig. 1. Electronic level structure calculated for Nd^{3+} ions in $NdNi_5$ in $|J,J_z>$ space under influence of molecular field and CEF with parameters taken from [13],[15].
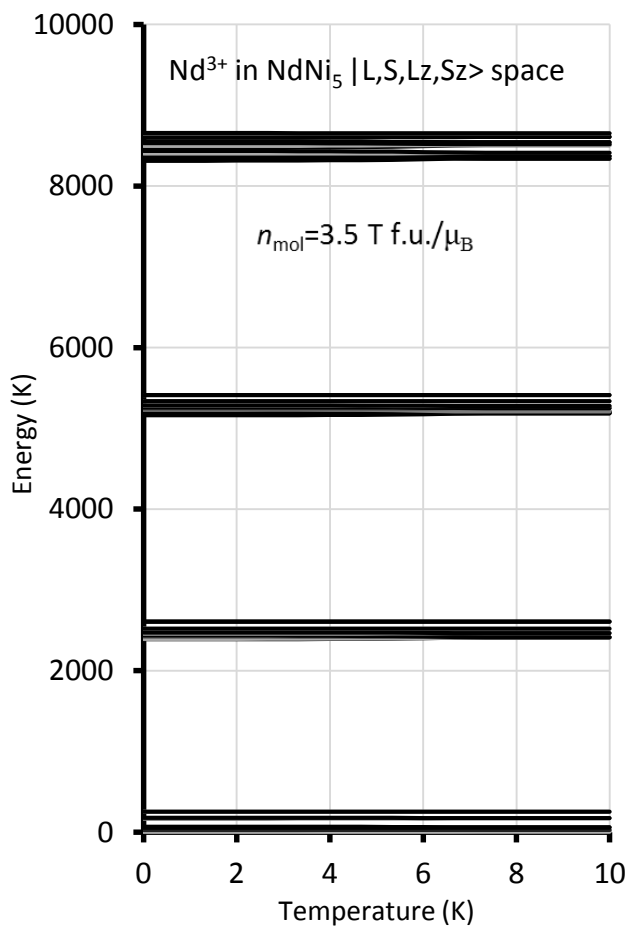

Fig. 2. Electronic level structure calculated for Nd^{3+} ions in $NdNi_5$ in $|L,S,L_z,S_z>$ space under influence of molecular field and CEF with parameters taken from [13],[15].
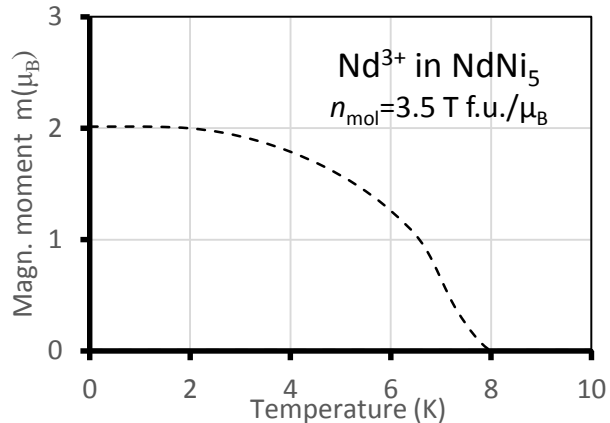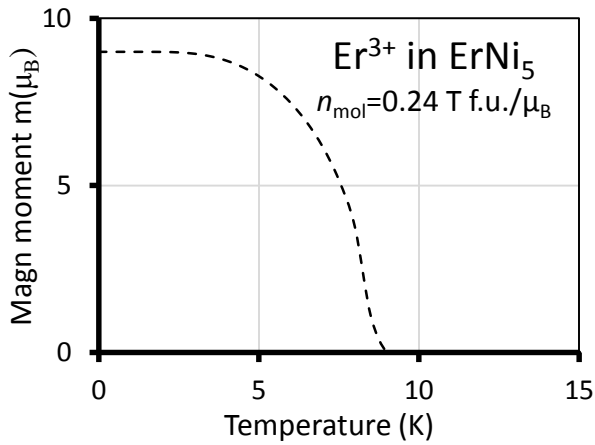

Fig. 3. Magnetic moment vs. temperature of Nd^{3+} ions in $NdNi_5$ under influence of molecular field and CEF with parameters taken from [13],[15]
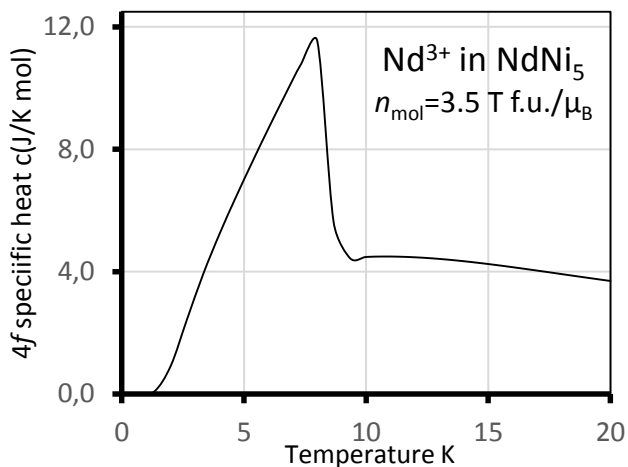
Fig. 4. $4f$ components of molar specific vs. temperature of Nd^{3+} ions in $NdNi_5$ under influence of molecular field and CEF with parameters taken from [13],[15] .
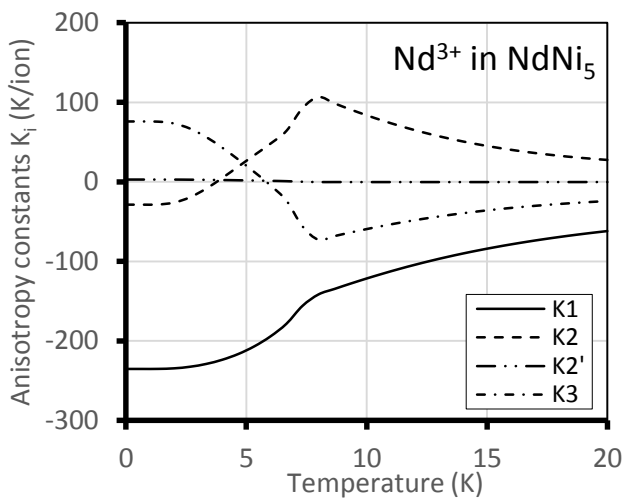
Fig. 5. Magnetocrystalline anisotropy constants vs. temperature, calculated for Nd^{3+} ions in $NdNi_5$ under influence of molecular magnetic field and CEF with parameters taken from [13],[15] n_{mol}=3.5 T f.u./μ_B.
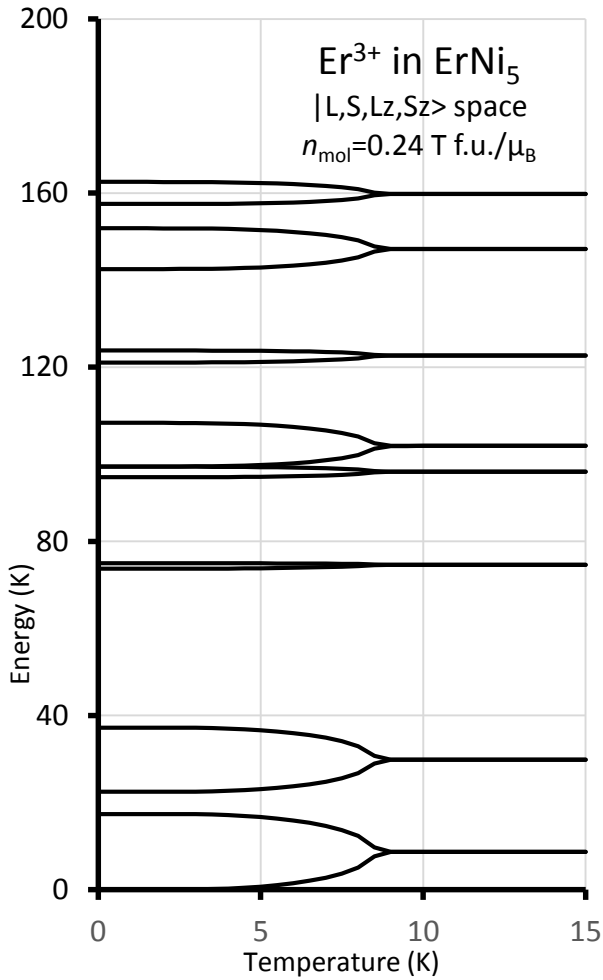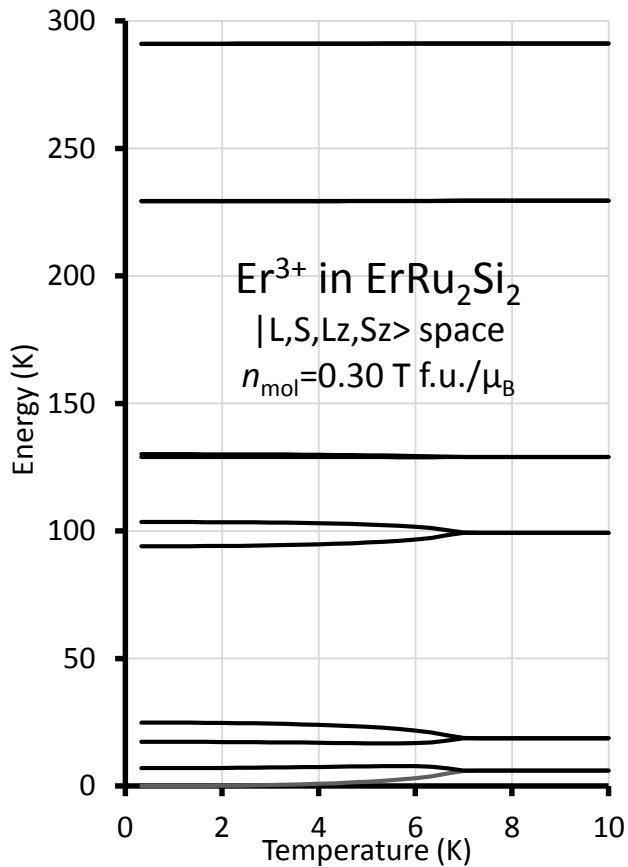
Fig. 6. Part of electronic level structure, near ground state, calculated for Er^{3+} ions in $ErNi_5$ in $|L,S,L_z,S_z>$ space under influence of molecular field and CEF with parameters taken from [15].
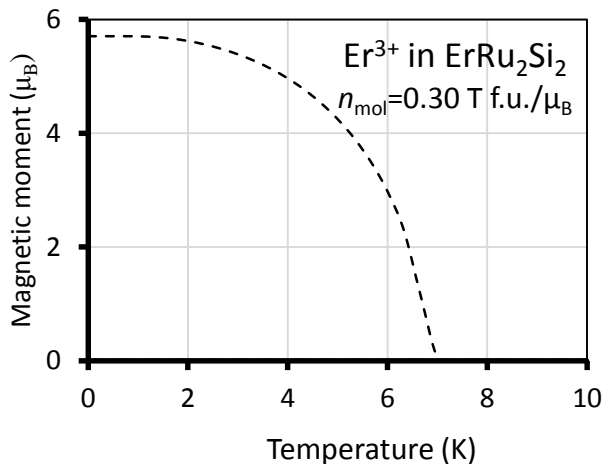

Fig. 7. Magnetic moment vs. temperature of Er^{3+} ions in $ErNi_5$ under influence of molecular field and CEF with parameters taken from [13],[15].
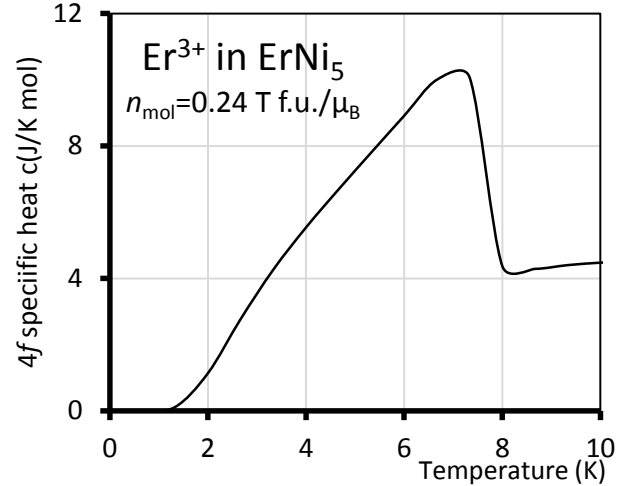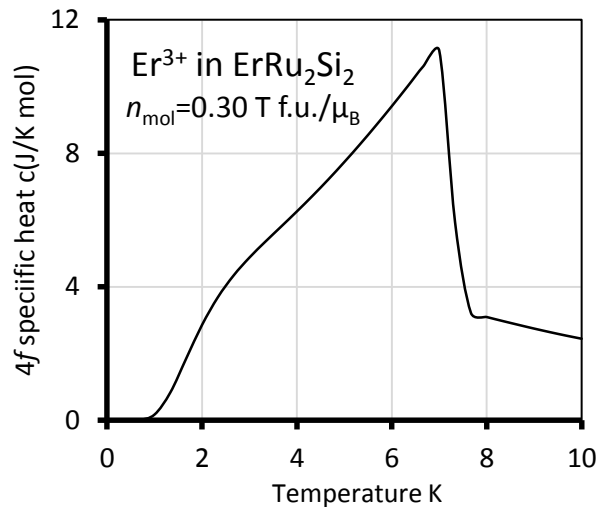

Fig. 8. $4f$ components of molar specific vs. temperature of Er^{3+} ions in $ErNi_5$ under influence of molecular field and CEF with parameters taken from [15].
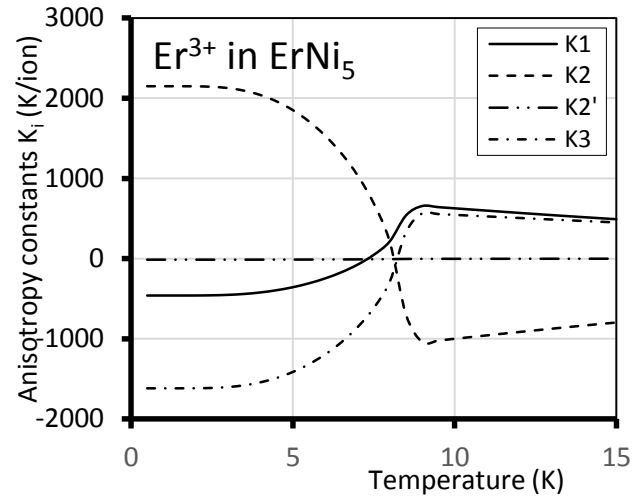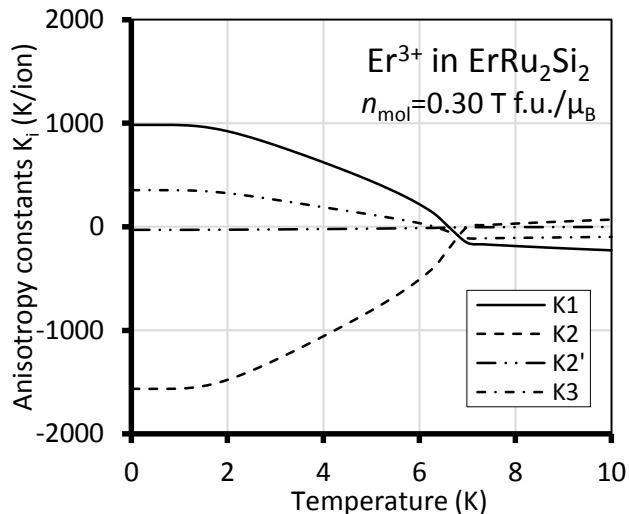

Fig. 9. Magnetocrystalline anisotropy constants vs. temperature, calculated for Er^{3+} ions in $ErNi_5$ under influence of molecular magnetic field and CEF with parameters taken from [15] n_{mol}=0.24 T f.u./μ_B

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3.2. Results for RRu_2Si_2 family of compounds

a. Results of calculations of Er^{3+} ions on $ErRu_2Si_2$ solid compound according to parameters: B^0_2=1.6K, B^0_4=-5mK, B^4_4=-4.5mK, B^6_0=-5μK, B^4_6=-0.52mK. Taken from: [16]

b. Results of calculations of Pr^{3+} ions on $PrRu_2Si_2$ solid compound according to parameters: B^0_2=-22K, B^0_4=0.22K, B^4_4=0.20K, B^0_6=-12mK, B^4_6=-45mK. Taken from: [18]

c. Results of calculations of Ce^{3+} ions on $CeRu_2Si_2$ solid compound according to parameters: B^0_2=1.07meV, B^0_4=0.015meV, B^4_4=0.59meV. Taken from: [19]
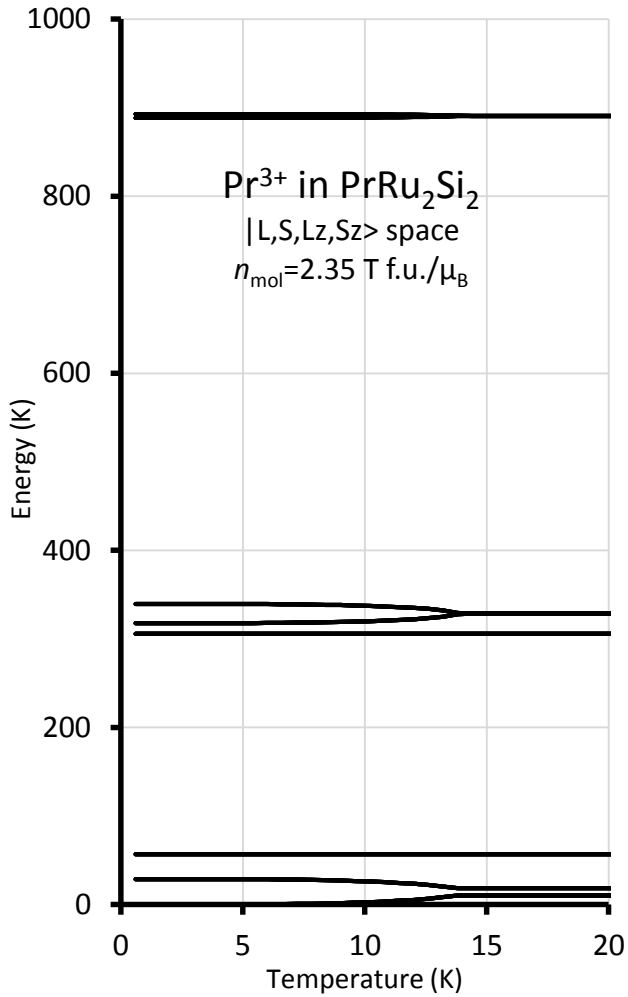

Fig. 10. Part of electronic level structure, near ground state, calculated for Er^{3+} ions in $ErRu_2Si_2$ in $|L,S,L_z,S_z>$ space under influence of molecular field and CEF with parameters taken from [16].
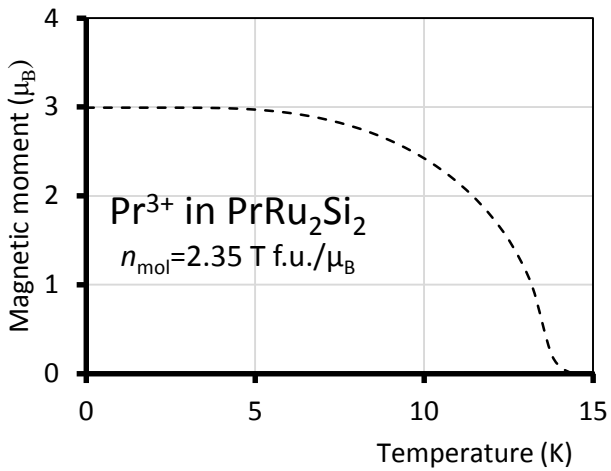

Fig. 11. Magnetic moment vs. temperature of Er^{3+} ions in $ErRu_2Si_2$ under influence of molecular field and CEF with parameters taken from [16].
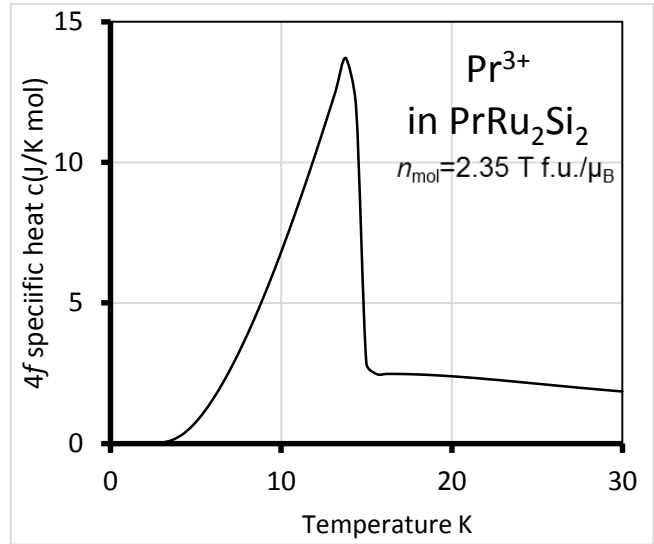

Fig. 12. 4f components of molar specific vs. temperature of Er^{3+} ions in $ErRu_2Si_2$ under influence of molecular field and CEF with parameters taken from [16].

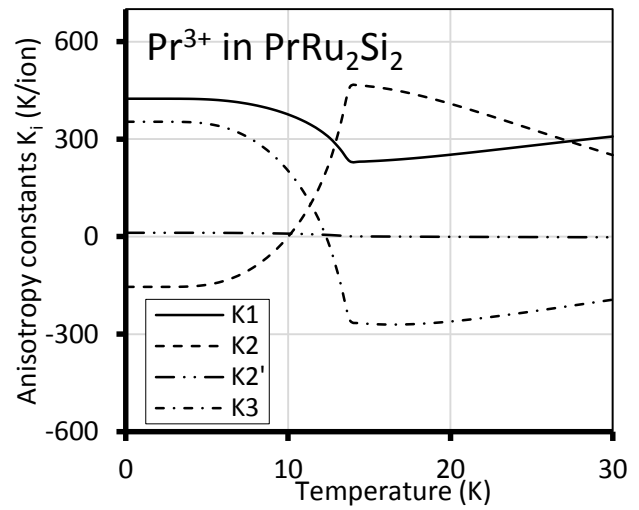Fig. 13. Magnetocrystalline anisotropy constants vs. temperature, calculated for Er^{3+} ions in $ErRu_2Si_2$ under influence of molecular magnetic field and CEF with parameters taken from [16]

Fig. 14. Part of electronic level structure, near ground state, calculated for Pr^{3+} ions in PrRu$_2$Si$_2$ in |L,S,L$_z$,S$_z$> space under influence of molecular field and CEF with parameters taken from [18].

Fig. 15. Magnetic moment vs. temperature of Pr^{3+} ions in PrRu$_2$Si$_2$ under influence of molecular field and CEF with parameters taken from [18].

Fig. 16. 4f components of molar specific vs. temperature of Pr^{3+} ions in PrRu$_2$Si$_2$ under influence of molecular field and CEF with parameters taken from [18].

Fig. 17. Magnetocrystalline anisotropy constants vs. temperature, calculated for Pr^{3+} ions in PrRu$_2$Si$_2$ under influence of molecular magnetic field and CEF with parameters taken from [18]
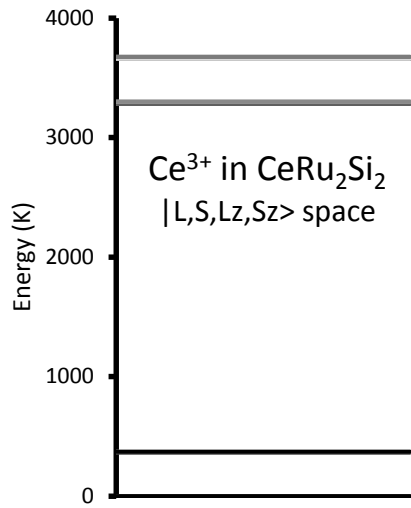
Fig. 18. Electronic level structure calculated for Ce^{3+} ions in $CeRu_2Si_2$ in $|L,S,L_z,S_z>$ space with CEF parameters taken from [19].
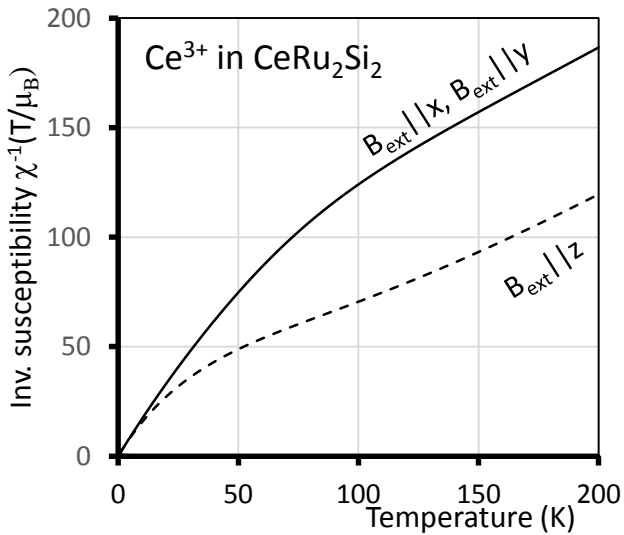

Fig. 19. Inverse plot of magnetic susceptibility calculated for different directions of external magnetic field for Ce^{3+} ions in $CeRu_2Si_2$ – calculated in $|L,S,L_z,S_z>$ space under influence with CEF parameters taken from [19].

3.3. Results for $R_2Fe_{14}B$ supermagnet family of compounds

a. Results of calculations for the famous compound $Nd_2Fe_{14}B$ with Nd^{3+} ions on 2 crystal lattice positions. We use average values recalculated from parameters $A^0_2=450K/a_0^2$, $B^0_4=-45K/a_0^4$, $A^0_6=-0.1K/a_0^6$ taken from [20].

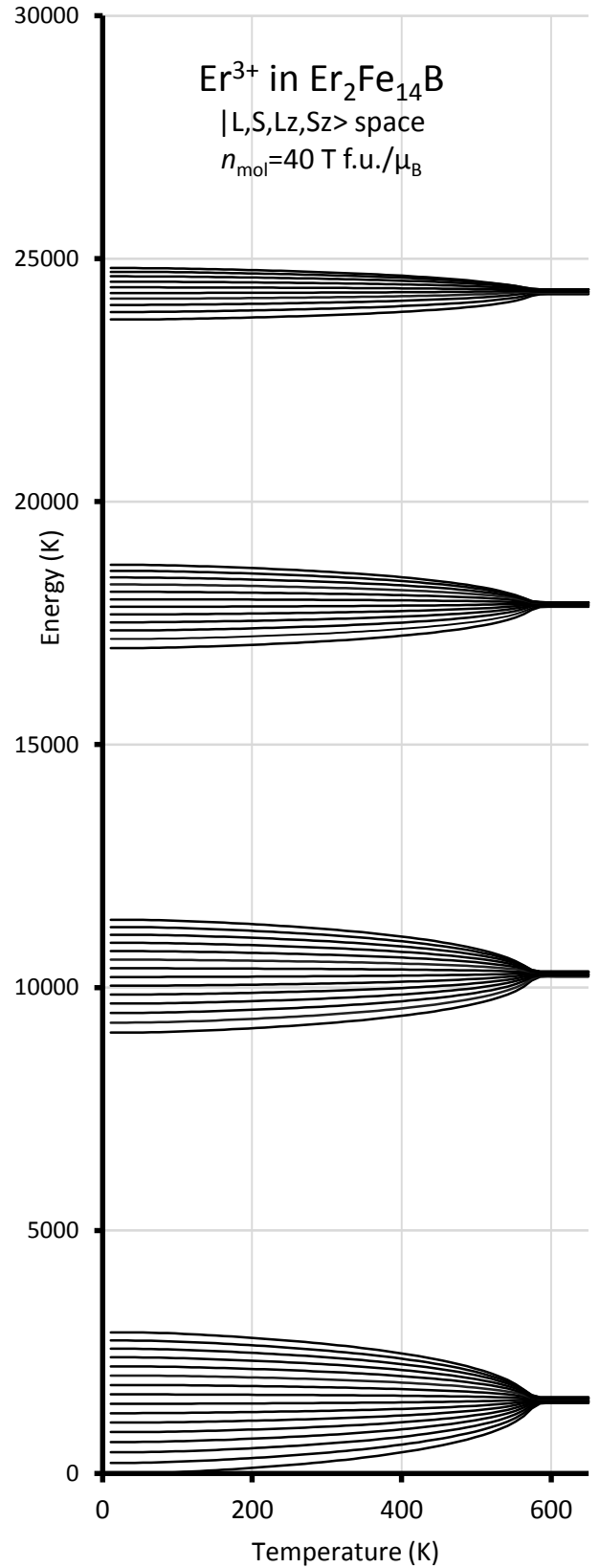b. Calculations results for Er^{3+} ions in $Er_2Fe_{14}B$ according to parameters: $B^0_2=0.562K$, $B^2_2=-0.417K$, $B^0_4=-1.38mK$, $B^0_6=-7.9\mu K$. Taken from [21]

Fig. 20. The full calculated fine electronic structure of Er^{3+} ions in $Er_2Fe_{14}B$ in $|L,S,L_z,S_z>$ space under influence of molecular field and CEF with parameters taken from [20].
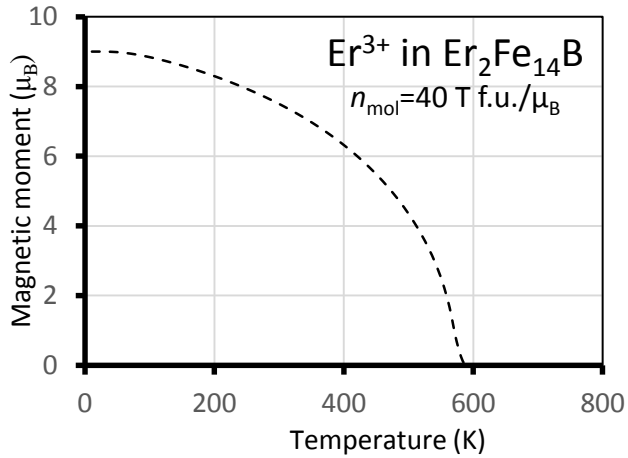
Fig. 21. Magnetic moment vs. temperature of Er^{3+} ions in $Er_2Fe_{14}B$ under influence of molecular field and CEF with parameters taken from [20].
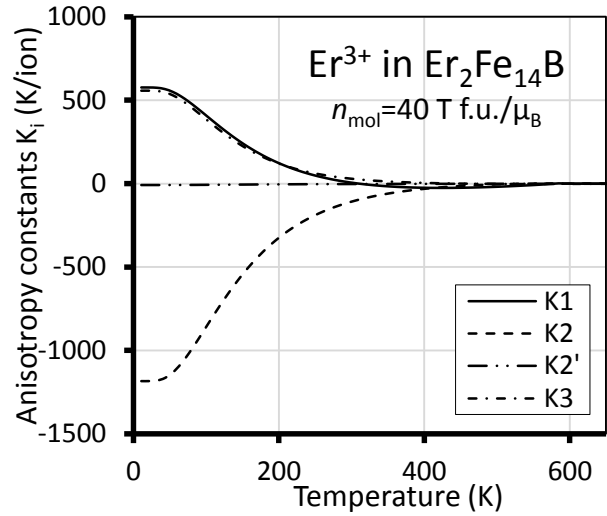

Fig. 23. Magnetocrystalline anisotropy constants vs. temperature, calculated of Er^{3+} ions in $Er_2Fe_{14}B$ under influence of molecular magnetic field and CEF with parameters taken from [20]

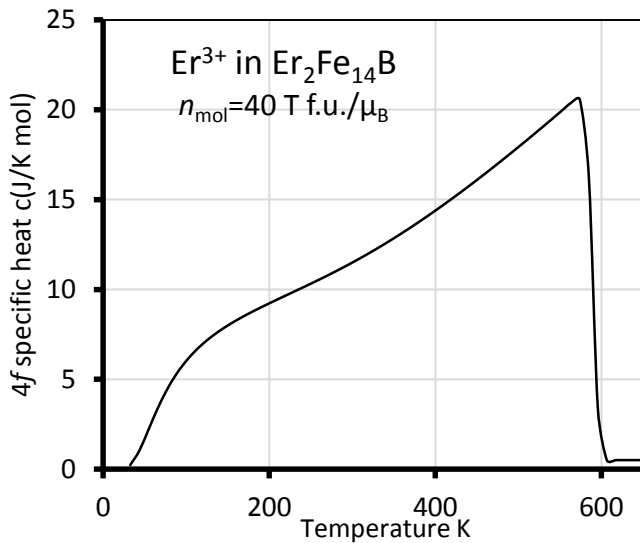Fig. 22. 4f components of molar specific vs. temperature of Er^{3+} ions in $Er_2Fe_{14}B$ under influence of molecular field and CEF with parameters taken from [20].
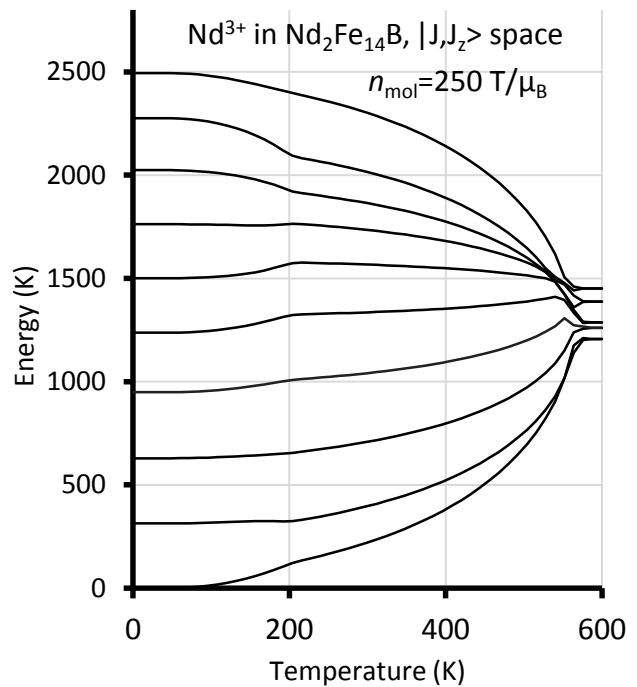

Fig. 24. The lowest multiplet splitting structure below T_C of Nd^{3+} ions in $Nd_2Fe_{14}B$ calculated in $|J,J_z>$ space under influence of molecular field and CEF with parameters taken from [21].
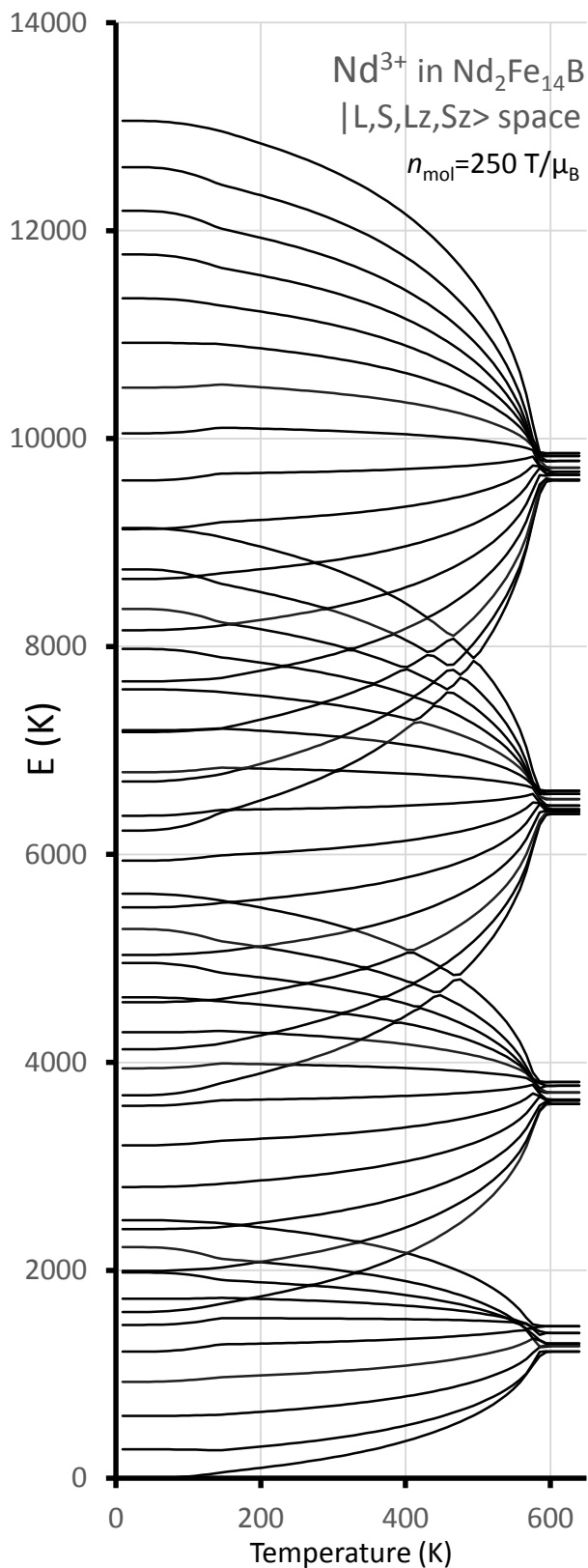
Fig. 25. The full calculated fine electronic structure of Ndr^{3+} ions in Nd$_2$Fe$_{14}$B in |L,S,L$_z$,S$_z$> space under influence of molecular field and CEF with parameters taken from [21].
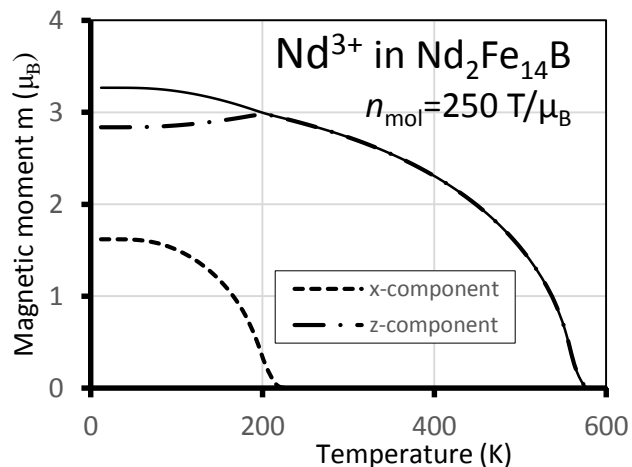

Fig. 26. Total magnetic moment ad its directional components vs. temperature of Nd^{3+} ions in Nd$_2$Fe$_{14}$B under influence of molecular field and CEF with parameters taken from [21].
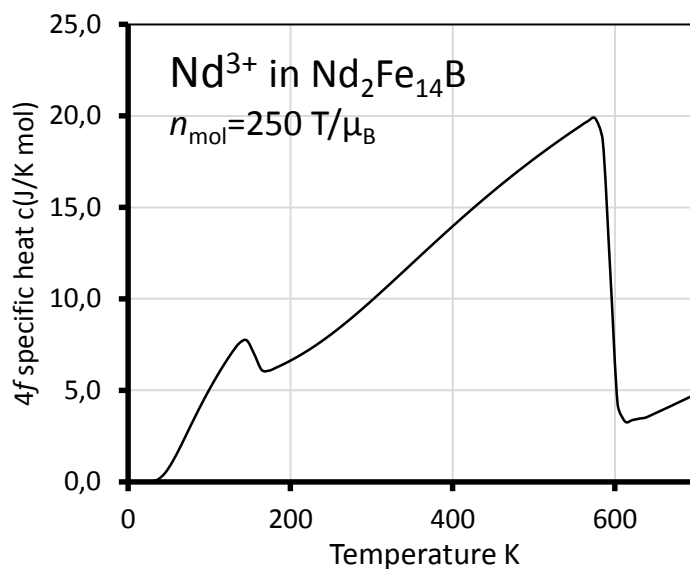

Fig. 27. 4f components of molar specific vs. temperature of Nd^{3+} ions in Nd$_2$Fe$_{14}$B under influence of molecular field and CEF with parameters taken from [21].
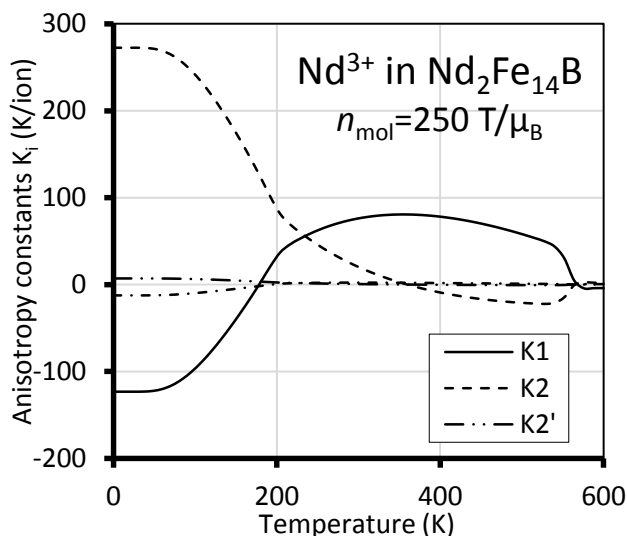
Fig. 28. Magnetocrystalline anisotropy constants vs. temperature, calculated of Er^{3+} ions in $Er_2Fe_{14}B$ under influence of molecular magnetic field and CEF with parameters taken from [21]

5. Conclusions

Selected calculations, based on parameters taken from scientific publications [11-21] were performed using ATOMIC MATTERS MFA computation system. All calculations provide some general conclusions:

In all cases, the |L,S,Lz,Sz> base is better for precise magnetism calculations and spectra recognition.

For some RE cases, the |J.Jz> base is not adequate, especially for crystals containing Ce^{3+} and Sm^{3+} ions.

Calculations on complex number matrices always give more precise spectra information. Full, correct directional magnetic information is provided by calculations on complex number matrices only.

In general, the most commonly used calculation base |J.J_z> and real number matrix Hamiltonian should be chosen for calculation speed reasons only because it offers approximate results with intermediate scientific value.

Working with ATOMIC MATTERS MFA revealed its high usefulness. The visual form of calculations results, full 3D interactive CEF potential visualization, intuitive tools for convention and unit recalculation, and the ability to compare data results all allow the user to utilize the power of the application very effectively. In conclusion, we confirm that ATOMIC MATTERS MFA is a unique application that combines a package of tools for correctly describing the physical properties of atomic-like electron systems subjected to electromagnetic interactions in real materials. This is accurate tool for properties calculations of ions under influence of the electrostatic potential of definable symmetry and both external and inter-ionic magnetic fields taken as a mean field approximation in magnetically ordered state. The interface of ATOMIC MATTERS MFA systems contains interactive, advanced visualization methods on interactive 3D and 2D plots. Hierarchical tab structure for parallel work, calculations speed and convenient comparison of many calculation results make the ATOMIC MATTERS MFA the effective tool for predictions of properties of novel magnetic materials for new unique applications.

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