Research Article

The Jour Multi Rese, 3(2), 2023, 7-13

The Journal of Multidisciplinary Research (TJMDR)

Content Available at www.saap.org.in **ISSN: 2583-0317**

PHASE TRANSITIONS OF A MIXED SPIN FERRIMAGNET IN HIGH TEMPERATURES

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Received: 19 Mar 2023 Revised: 14 May 2023 Accepted: 06 June 2023

Abstract

In this research paper molecular mean field theory (MMFT) has been investigated based on Gibbs-Bogoliubov free energy function of a ferrimagnetic mixed spin-3 and spin-5/2 Blume-Capel model with different magnetic crystal fields. The free energy of the proposed ferrimagnet has been evaluated depending on the trial Hamiltonian operator. Minimizing the free energy, one may induce characteristic features of the longitudinal magnetizations, phase transitions and spin compensation temperatures, in the ranges of low temperatures, respectively. In particular, we study the effect of crystal field domains on the critical phenomena for the proposed model. The sublattice magnetization dependence of free energy function has been discussed as well. Our results predict the existence of multiple spin compensation sites in the disordered Blume-Capel Ising system for a simple cubic lattice.

Keywords: Molecular mean field theory; Ferrimagnetic phase transition; Crystal field domain; Spin free energy function; Curie temperature.

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DOI: https://doi.org/10.37022/tjmdr.v3i2.450

Produced and Published by

South Asian Academic Publications

Introduction

Because of the increasing demands being placed on the performance of magnetic solids, there has been much interest in the magnetic properties testing of molecule-based magnets. The crystalline nonmetallic compounds with A_pB_{1-p} where A and B are different magnetic atoms, which are ferrimagnets due to a strong negative A–B exchange interaction, have found important applications in recording media, and permanent magnets[1-6]. It is important to mention that in rare earths of the paramagnets the R-Mn $(R \equiv Tb - Er; Erbium - Terbium)$ couplings are dense enough to align the manganese moments of the Mn-R-Mn slabs, which gives the ferromagnetic assemblies of Nd- and $SmMn_6Ge_6$, and the ferrimagnetic prearrangement detected in RMn_6Sn_6 compounds at room temperature[7,8]. Thus, a ferrimagnetic behavior at high temperature in Tb has to be related to a dominant negative Tb-Mn exchange interaction[7]. Researchers, in this respect, observed the magnetic behavior of which can be described as" bootstrap ferrimagnetism", i.e., at high temperature these composites visibly act as archetypal ferrimagnets. M. Karimou et al.[9] have investigated the crystal field and external magnetic field effects on the magnetization of the mixed-spin (7/2, 5/2) ferrimagnetic according to the Ising model that can be by Monte Carlo simulation and mean-field calculations. The authors have induced compensation temperatures for such a system where the global magnetization vanishes. Particularly, a bilayer magnetic film with an ordered Ising-type Hamiltonian has been examined taking into consideration an interlayer antiferromagnetic coupling. It is essential, in this work, a mixed-spin Blume-Capel Ising model, to be examined consisting of spin-3 and spin-5/2. Ground-state phase diagrams are useful to check the reliability of numerical results for these diagrams at low temperatures and high temperatures, respectively. So, it allows identifying regions induce interesting magnetic phenomena[10-19]. The goal of this research paper is to construct the ground-state phase diagram and studied sublattice magnetizations of the disordered alloy with various magnitudes of the crystal fields, throughout the framework of molecular mean-field approximation (MMFA). A Landau-Bogoliubov expression of the free energy in the order parameter is required.

Methodology

It has been investigated the nearest neighbor Blume-Capel Ising model in zero field on a lattice has two sublattices *A,B* having *N* sites, each site having z nearest neighbor. The exchange interaction between A and B atoms is proposed to be ferrimagnetic. Now, the proposed system is expressed by the Hamiltonian operator as [11,12],

$$H = -\sum_{i,j} J_{ij}\mu_i^A \mu_j^B - D_A \sum_i (\mu_i^A)^2 - D_B \sum_j (\mu_j^B)^2 \quad (1)$$

where the sites of sublattice *A* are occupied by spins μ_i^A including the values $\pm 3, \pm 2, \pm 1, 0$, and the sites of sublattice *B* occupied by spins μ_j^B with the values of $\pm 1/2, \pm 3/2, \pm 5/2$. $D_A/|J|$, and $D_B/|J|$, are the crystal fields, i.e., magnetic anisotropies acting on tthe spin-3, spin-5/2, respectively. J_{ij} is thetexchange interaction between spins at sites *i* and *j*. A systematic way of evaluating the MFM for a microscopic Hamiltonian is to start from the Bogoliubov inequality as[20],

$$f \le \varphi = f_o + \langle H - H_o \rangle_o \quad (2)$$

where f is the free energy function of the present system, H_o is a trial Hamiltonian operator depending on variational parameters, and f_o the corresponding free energy function. In this research paper we consider the suitable choices of a trial Hamiltonian operator is[19,20],

$$H_o = -\sum_i [K_A \mu_i^A + D_A (\mu_i^A)^2] - \sum_j [K_B \mu_j^B + D_B (\mu_j^B)^2] \quad (3)$$

K_A and K_B are the two variational parameters are connected to the two different spins, respectively. So, one obtains the free energy of the proposed system that Eq.(2) becomes,

$$\begin{aligned} f = -\frac{1}{2\beta}\{ &\ln[2e^{9\beta D_A}\cosh(3\beta K_A) + 2e^{4\beta D_A}\cosh(2\beta K_A) + 2e^{\beta D_A}\cosh(\beta K_A) + 1] + \\ &\ln[2e^{25/4\beta D_B}\cosh(\tfrac{5}{2}\beta K_B) + 2e^{9/4\beta D_B}\cosh(\tfrac{3}{2}\beta K_B) + 2e^{1/4\beta D_B}\cosh(\tfrac{1}{2}\beta K_B)]\} + \\ &1/2(-zJm_A m_B + K_A m_A + K_B m_B) \end{aligned} \quad (4)$$

Minimizing this expression with respect to K_A and K_B giving self-consistent formulae for the mean magnetic moments, as,

$$m_A \equiv \langle \mu_i^A \rangle_o = \frac{1}{2}\frac{6\sinh(3\beta K_A) + 4e^{-5\beta D_A}\sinh(2\beta K_A) + 2e^{-8\beta D_A}\sinh(\beta K_A)}{\cosh(3\beta K_A) + e^{-5\beta D_A}\cosh(2\beta K_A) + e^{-8\beta D_A}\cosh(\beta K_A) + 0.5e^{-9\beta D_A}} \quad (5)$$

$$m_B \equiv \langle \mu_j^B \rangle_o = \frac{1}{2}\frac{5\sinh(\frac{5}{2}\beta K_B) + 3e^{-4\beta D_B}\sinh(\frac{3}{2}\beta K_B) + e^{-6\beta D_B}\sinh(\frac{1}{2}\beta K_B)}{\cosh(\frac{5}{2}\beta K_B) + e^{-4\beta D_B}\cosh(\frac{3}{2}\beta K_B) + e^{-6\beta D_B}\cosh(\frac{1}{2}\beta K_B)} \quad (6)$$

and,

$$K_A = zJm_B \qquad , K_B = zJm_A \quad (7)$$

One finds the ferrimagnetic compensation behavior of the considered system can be obtained by requiring the total magnetization as being equal to zero for different values of crystal fields; though the reduced magnetization of the anticipated structure are not equal to zero[19, 20], that,

$$M = \frac{1}{2}(m_A + m_B) \quad (8)$$

Results and Discussion

The mixed spin-3 and spin-5/2 Blume-Capel Ising model expose nine phases with various values of $\{m_A, m_B, \lambda_A, \lambda_B\}$, i.e., the ordered ferrimagnetic phases are,

$$O_1 \equiv \{-3,\frac{5}{2},9,\frac{25}{4}\}, or, O_1 \equiv \{3,-\frac{5}{2},9,\frac{25}{4}\}, O_2 \equiv \{-2,\frac{5}{2},4,\frac{25}{4}\}, or, O_2 \equiv \{2,-\frac{5}{2},4,\frac{25}{4}\},$$
$$O_3 \equiv \{-1,\frac{5}{2},1,\frac{25}{4}\}, or, O_3 \equiv \{1,-\frac{5}{2},1,\frac{25}{4}\}, O_4 \equiv \{-3,\frac{3}{2},9,\frac{9}{4}\}, or, O_4 \equiv \{3,-\frac{3}{2},9,\frac{9}{4}\},$$
$$O_5 \equiv \{-2,\frac{3}{2},4,\frac{9}{4}\}, or, O_5 \equiv \{2,-\frac{3}{2},4,\frac{9}{4}\}, O_6 \equiv \{-1,\frac{3}{2},1,\frac{9}{4}\}, or, O_6 \equiv \{1,-\frac{3}{2},1,\frac{9}{4}\},$$
$$O_7 \equiv \{-3,\frac{1}{2},9,\frac{1}{4}\}, or, O_7 \equiv \{3,-\frac{1}{2},9,\frac{1}{4}\}, O_8 \equiv \{-2,\frac{1}{2},4,\frac{1}{4}\}, or, O_8 \equiv \{2,-\frac{1}{2},4,\frac{1}{4}\},$$
$$O_9 \equiv \{-1,\frac{1}{2},1,\frac{1}{4}\}, or, O_9 \equiv \{1,-\frac{1}{2},1,\frac{1}{4}\},$$

and disordered phases:

$D_1 \equiv \{0,0,0,\frac{25}{4}\}, D_2 \equiv \{0,0,0,\frac{9}{4}\}, D_3 \equiv \{0,0,0,\frac{1}{4}\}$. The parameters λ_A and λ_B are defined as:

$$\lambda_A = \langle(\mu_i^A)^2\rangle, \qquad \lambda_B = \langle(\mu_j^B)^2\rangle \tag{9}$$

For evaluating the corresponding ground-state energies per site for each of the indicated phases above. One can construct the ground-state phase diagram of the system with z=6, as shown in Fig.1.

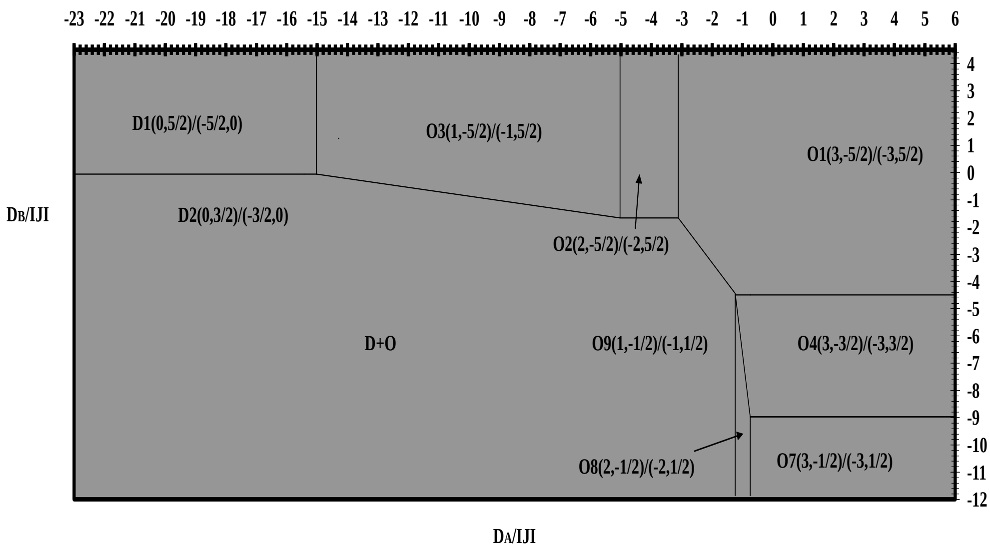

Fig.1. Ground- state phase diagrams that considered model with the nearest neighbor(z=6) and different crystal fields D_A and D_B. The ordered and disordered phases: $O_1, O_2, O_3, O_4, O_7, O_8, O_9, D_1, D_2, and (D+O) : O_5, O_6, D_3$, ,are separated by thin lines, respectively.

We find the ground-state phase diagram structure, for the temperature requirement of the interpenetrated lattices magnetization m_A and m_B, solved numerically by the coupled Eqs.((5)-(7)). For a simple cubic lattice, as shown in Fig.2, the observable range $-5.0 \le D_A/|J| \le -2.5$, that the heat dependence of m_B may exhibit a rather smooth decrease from the saturation value at $k_BT/|J| = 0$. When the value of $D_A/|J|$ approaches the critical value, the phenomenon is clearly enhanced. Particularly, at the critical value of the A-atom anisotropy, when $k_BT/|J| = 0$, the saturation value of m_A is 1.0, indicating that in the ground state the spin configuration of the system consisting of the mixed phases $s_j^A = \pm\frac{3}{2}$, and $s_j^A = \pm\frac{1}{2}$, are with equal probability. So, one should notice that a new behavior induced in the present model, not predicted in the Ne'el theory of ferrimagnetism[21], when a value of $D_A/|J|$ approaches the critical one, i.e., $D_A/|J| = -5.0$.

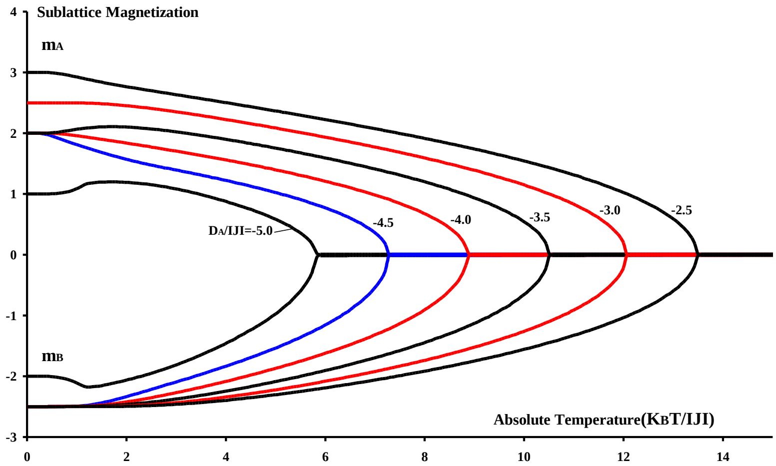

Fig.2. the submagnetizations m_A ,m_B based on temperature variations for the mixed ferrimagnet(z=6), when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -1.5$

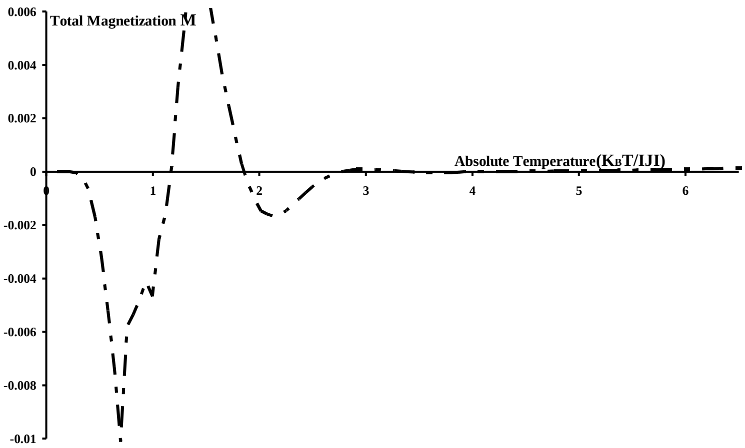

Fig.3. A closer look at M on the basis of different heat signatures. for the same considered system, but with z=6, when $D_A/|J| = -3.0$ and $D_B/|J| = -2.995$.

Besides, we present an intriguing characteristic of compensating temperatures for a simple cubic lattice at various anisotropies. $D_A/|J| = -3.0$, $D_B/|J| = -2.995$. As is noticed from the Fig.3, The compensation magnetization seems to be more organized m_A than the submagnetization beneath compensating heat in the region where the system may display three compensating sites. These sublattice magnetizations are remained inadequate, so there is a remaining magnetization. As the temperature is increased, at certain values of crystal fields, i.e., magnetic anisotropies $D_A/|J|$, $D_B/|J|$ acting on the sublattices atoms, the orientation of the residual magnetization may switch. Because of the entropy of certain spins can flip their directions, the sublattice magnetization m_B becomes more well-organized than the submagnetization m_A, for the temperatures above compensation one. However, there is an intermediately point such that the cancellation is complete, so a compensation temperature is induced[20]. It is worth mentioning that the molecular MFT for ferrimagnetictcase, predicts the presence of abcompensation pointiin the orderedtphase whereithe total moment become vanish [5, 6].

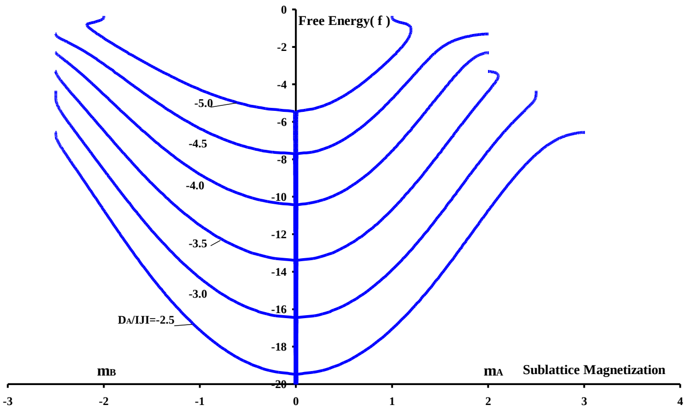

Fig.4. Free energy dissimilarities of the submagnetizations for a z=6 of the mixed-spin ferrimagnet for several values of $D_A/|J|$, when the magnitude of $D_B/|J| = -1.5$.

we have inspected the action of free energy on thermodynamic phase steadiness of the system under study. Free energy of the present system has been calculated according to Eq.(4), so the free energy behaviors are shown in Fig.4, for a simple cubic lattice. The behavior of a ferrimagnetic or antiferromagnetic state(at a compensation point $T < T_C$; where T_C is the transition temperature) and paramagnetic one(at transition temperature $T > T_C$), is based on the curve of free energy exhibits an inflexion that correlates to a discontinuity, however at a critical anisotropy value, the system's freecenergy istcontinuous[20,21]. As a result, the magnetizationicurves constantly decrease to zero, separating the ferrimagneticmphase from the paramagneticsphase; this occurrence is termed as phaseitransition. of the second-order or the Curie point. Whenia magnetization fallsvto zero or some value, however, a first-order phaseotransition happens, or perhaps thentemperature at whichnthe magnetization jump occurs[20]. The features shown in Fig.4, is convenient with those derived from Fig2.

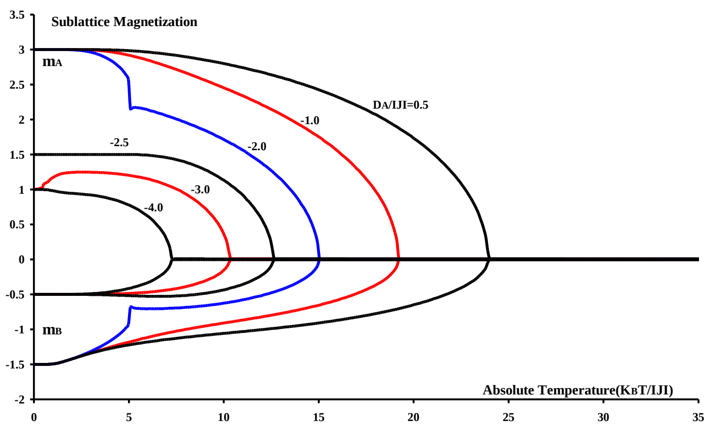

Fig.5. Temperature dependences of the sublattices magnetizations m_A, m_B for the mixed ferrimagnet(z=6), when the value of D_A is changed, for fixed $D_B = -20.0$

In Figs.5,6, it has been plotted the sublattices magnetizations versus temperature, for two values of $J=-2.5,-3.5$, when $D_B=-20.0$. Our proposed system experiences second-order phase transition temperatures are $T_C=24K^o$, and $T_C=45.51K^o$, for $J=-2.5,-3.5$, respectively. This is evident that the system can be examined in high temperatures, when the exchange interaction couplings between ions become $J<-1.0$. Accordingly, in the present system the transition temperature T_C, is proportional to the number of magnetic neighbors around a given ion and to the magnitude of the interaction between two centres[22]. From Figs.6,7, the system is passed through second-order phase transitions and then it moves to first-order transitions when $D_A=1.0,0.5,-0.5,-1.0,-1.5,-2.5,-3.5,-4.5,-4.5,-5.5,-6.5$, for fixed $D_B=-20.0$, or when $D_B=1.0,0.5,-0.5,-1.0,-1.5,-2.5,-3.5,-4.5,-5.5$, for atfixed value of $D_A=-20.0$, respectively.

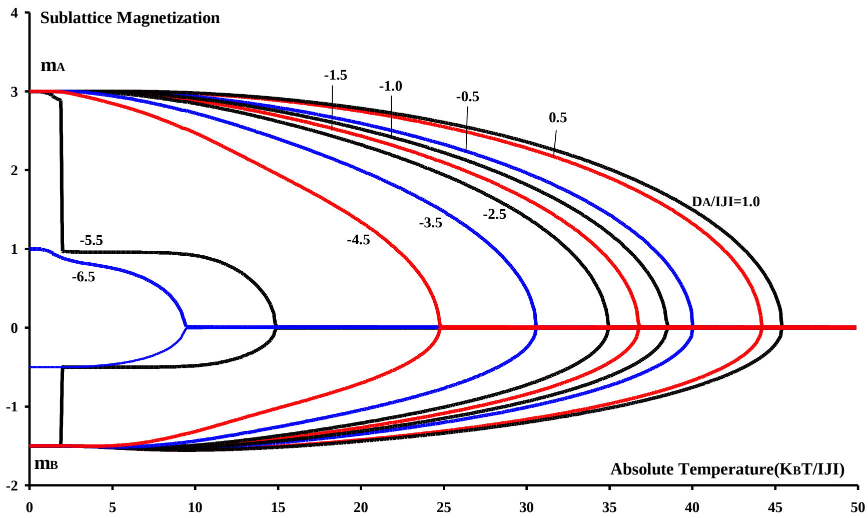

Fig.6. Temperature variations of the sub magnetizations m_A, m_B for the mixed ferrimagnet(z=6), where D_A is changed, for fixed $D_B=-20.0$

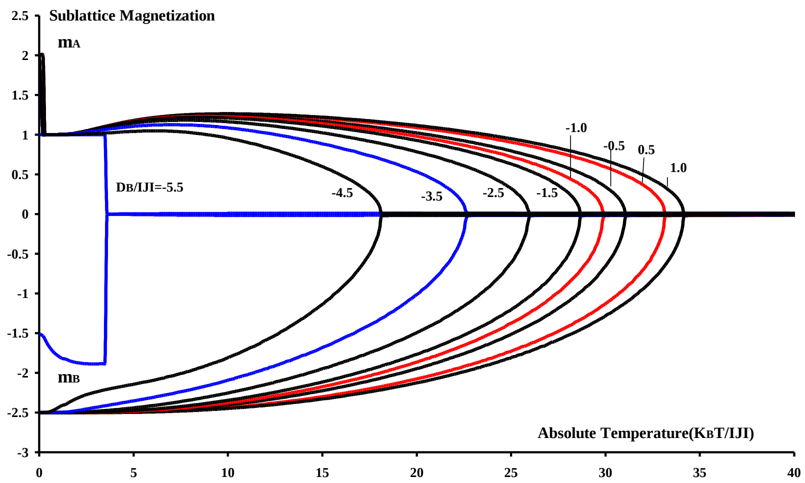

Fig.7. Temperature requirements of the sub magnetizations m_A, m_B for the mixed ferrimagnet(z=6), where D_B is changed, for fixed $D_A=-20.0$.

Conclusion

The ground-state phase diagrams of the mixed spin-3 and spin-5/2 Blume-Capel Ising ferrimagnetic system with different crystal fields, i.e., single-ion anisotropies have been constructed. The magnetic properties of the present lattices have been found by solving the general expressions numerically. So, the magnetization curves have exhibited characteristic features that it may produce a spin compensation phenomenon. One can compare our results with those of a mixed spin-2 and spin-5/2 on a square lattice[6]. The researchers presented a ground-state phase diagram and studied the influence of crystal fields. They discovered that increasing the number of interactions causes higher sophistication in the phase diagrams, allowing them to investigate locations where key magnetic phenomena may emerge. A theoretical study dealing with the mixed spin-2 and spin-3/2 Ising model, using mean field theory[20], it has determined the phase diagram. However, the proposed system may display three compensation points. It had been demonstrated that the decrease the magnetic anisotropy of B-atoms the decrease the transition temperature(see Fig.7). Our recent findings might be useful in sustaining and elucidating the distinguishing properties of a series of molecular-based magnets. The R-Mn links are robust enough just to recover and realign the manganese moments of the Mn-R-Mn slabs, giving rise to the ferromagnetic structures of Nd- and $SmMn_6Ge_6$, and the ferrimagnetic arrangement.

Conflict of Interest

The authors declare no conflict of interest

Funding

No Funding

Inform consent

Not Applicable

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