Magnetic properties of dendrimer structures with different coordination numbers: A Monte Carlo study

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ABSTRACT

We investigate the magnetic properties of Cayley trees of large molecules with dendrimer structure using Monte Carlo simulations. The thermal magnetization and magnetic susceptibility of a dendrimer structure are given with different coordination numbers, $Z=3$, 4, 5 and different generations $g=3$ and 2. The variation of magnetizations with the exchange interactions and crystal fields have been given of this system. The magnetic hysteresis cycles have been established.

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1. Introduction

In previous work [1–4], many progresses have been made in the analysis of structural properties of a special class of branched polymers, named dendrimers. The synthesis and magnetic properties of novel dendrimeric spin crossover Fe(III) complex of formula, where $L=$3,5-di(3,4,5-tris(tetradecyloxy) benzoyloxy) benzoyl-4-oxy-salicylidene-N′-ethyl-N-ethylene-di-amine have been studied for the first time by magnetic susceptibility, Electron Paramagnetic Resonance (EPR) and Mössbauer spectroscopy in the wide (2–300 K) temperature range [5]. Gadolinium (Gd^{3+}) based dendrimers with precise and tunable nanoscopic sizes are excellent candidates as magnetic resonance imaging contrast agents [6]. A novel inorganic–organic hybrid nanomaterial was prepared by anchoring (3-glycidyloxypropyl) trimethoxysilane at the surface of graphene oxide, further cross-linking with poly-amidoamine G-4 dendrimer, and final decoration with platinum nanoparticles [7]. The magnetic properties of cobalt nanoparticles with dendrimers as templates have been investigated [8]. Stable magnetic magnetite nanoparticles (Fe_3O_4 NPs) were synthesized using the chemical coprecipitation method of ferrous (Fe^{2+})/ferric (Fe^{3+}) mixed aqueous salt solutions in presence of well-defined biocompatible low generation (poly)amidoamine (PAMAM)-based dendrimers with end grafted n ethylene glycol ether ($n=1$, 2, 9) moieties, accessible by means of straightforward consecutive divergent synthesis methodologies including addition and amidation cycles [9]. The interactions between dendrimer-coated magnetite nanoparticles and the protein serum albumin have been investigated [10]. The dendrimer-magnetic nanoparticles may be looked upon as high-efficiency drug delivery system with the potential to achieve magnetic drug targeting and magnetic hyperthermia [11]. Dendrimers with terminal amino groups attached to the particle surface were used to bind chelating groups for lanthanides and actinides [12]. Polyamidoamine dendrimer was synthesized on the surface of amino silane modified magnetite nanoparticles [13]. A polyamidoamine dendrimer was grafted onto magnetic multi-walled carbon nanotubes to combine magnetic properties with a large surface functionalized with amino groups [14]. Chiral selector-functionalized magnetic microspheres have significantly potential in the recognition and separation of chiral compounds [15]. The nanostructured sensing interface was prepared with poly(dopamine)-modified magnetic nanoparticles which were covalently coated with four-generation ethylenediamine core polyamidoamine G-4 dendrimers and further decorated with platinum nanoparticles [16]. The magnetic properties of mixed spins Ising model on the Bethe lattice have been investigated using the Monte Carlo simulation [17,18]. In this work, we have studied the magnetic properties of a dendrimer. The model and formulation are presented in Section 2. Numerical details have been given in Section 3. The results and discussion are presented in Section 4. Finally, we have presented in Section 5 the conclusion.

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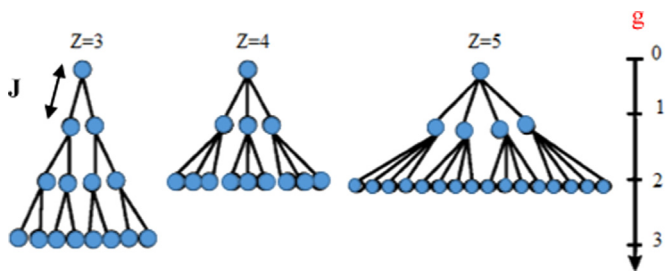   E-mail address: rachidmasrour@hotmail.com (R. Masrour).

Fig. 1. Schematic of three dendrimers, with $Z=3$, 4, and 5. The generation order, g, is as shown, $g=3$ (for $Z=3$), and $g=2$ (for $Z=4$, and 5).
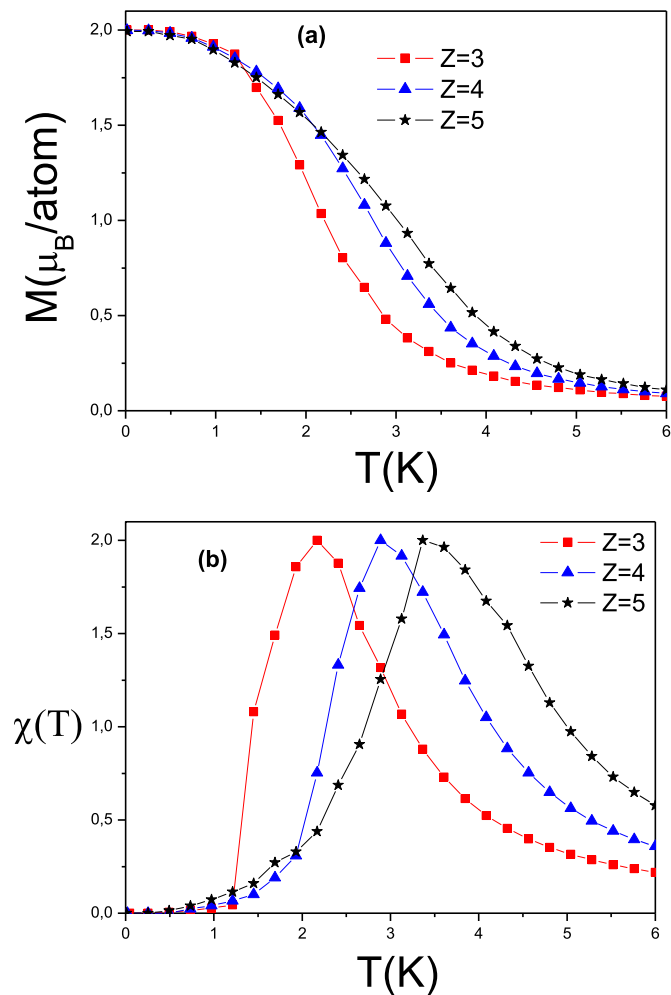

Fig. 2. The thermal magnetization (a) and magnetic susceptibility (b) for different coordination numbers, $Z=3$, 4 and 5 of a dendrimer structure with $\Delta/k_B=0.0$, $J/k_B=1.0$ K and $h=0.1$ T.

Fig. 3. The magnetization versus the exchange interaction for $T=1.0$ K (a) and 1.5 K (b) for different coordination numbers, Z of a dendrimer structure with $\Delta/k_B=0.0$ and $h=0.05$ T.

$$H = -J \sum_{<i,j>} S_i S_j - \Delta \sum_i S_i^2 - h \sum_i S_i \tag{1}$$

h is the external magnetic field and Δ represent the crystal field. The coupling J is the first exchange interactions parameter between the two magnetic ions. The values of spin moment are: $S = \pm 2; \pm 1; 0$.

2. Model and formulation

We consider a large molecules with dendrimer structure with different coordination numbers, Z, and different generations orders g such as given in Fig. 1 and it is given in Refs. [19,20]. Varying the branching ratio Z (or number of nearest neighbors, also known as coordination number), and the generation number (order) g can produce a large variety of such structures. It has also been proposed that controlling these two parameters is the key to controlling energy transport in such structures. The Hamiltonian of such a system with dendrimer structure includes first exchange interactions, external magnetic field and the crystal field has the form:
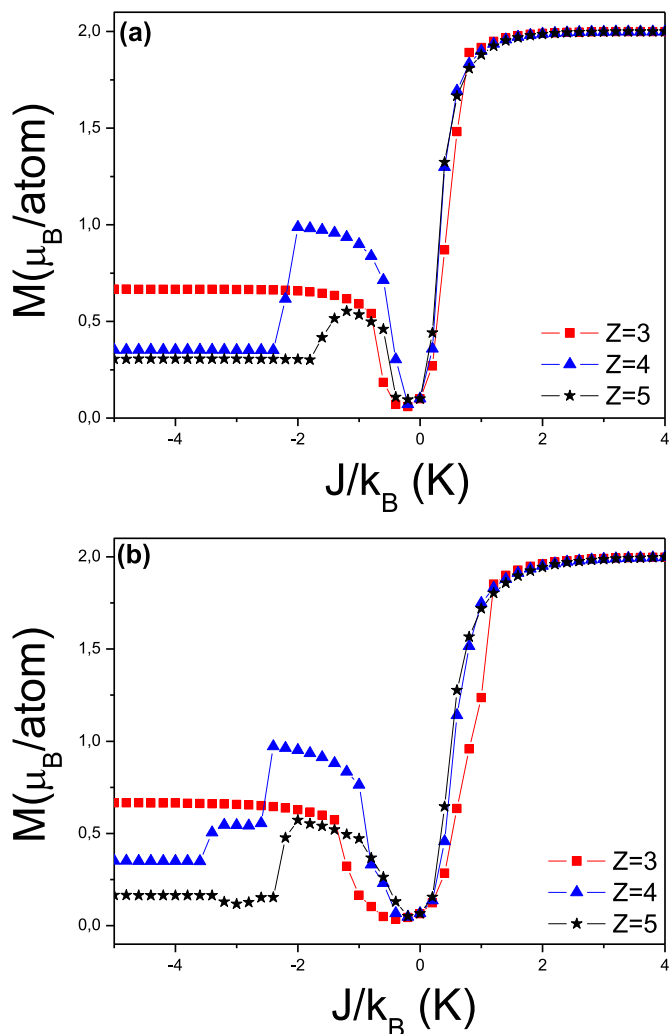
3. Numerical details

A dendrimer structure with different coordination numbers, Z, and different generations orders g is assumed to reside in the unit cells and the system consists of the total number of atoms is $N = \sum_{i=0}^{g} (Z-1)^i$ with g is the different generations orders of a dendrimer structure. Where N is the total number of sites. For the coordination numbers $Z=3$, 4 and 5, the obtained values of N are 15, 40 and 85 respectively such as given in Fig. 1. We apply a standard sampling method [21] to simulate the Hamiltonian given by Eq. (1). Cyclic boundary conditions on the system were imposed and the configurations were generated by sequentially traversing the lattice and making single-spin flip attempts. The flips are accepted or rejected according to a heat-bath algorithm under the Metropolis approximation. Our data were generated with 10^5