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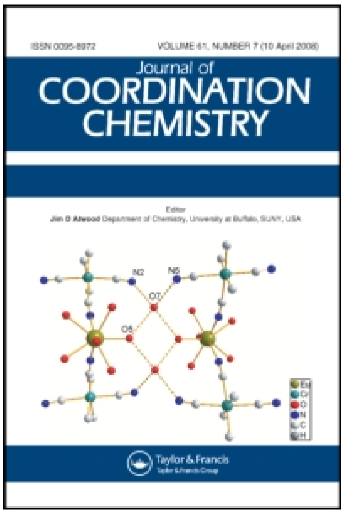

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Crystal structure and magnetic properties of a heteronuclear, gadolinium-zinc carboxylate complex

Bin Wu[a]; Wei-Min Lu[a]; Fang-Fang Wu[a]; Xiao-Ming Zheng[a]
[a] Institute of Catalysis, Zhejiang University, Hangzhou, P. R. China

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CRYSTAL STRUCTURE AND MAGNETIC PROPERTIES OF A HETERONUCLEAR, GADOLINIUM–ZINC CARBOXYLATE COMPLEX

BIN WU, WEI-MIN LU*, FANG-FANG WU and XIAO-MING ZHENG

Institute of Catalysis, Zhejiang University, Xixi Campus, Hangzhou, 310028, P. R. China

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A novel heteronuclear complex, $[Gd_2Zn_2L_{10}(bipy)(H_2O)_2]_2$ (HL = α-methylacrylic acid, bipy = 4,4′-bipyridine), was synthesized and characterized. Its structure, determined by X-ray diffraction, reveals a discrete octanuclear molecule, in which two Zn^{II} ions are linked by a bipy molecule and Gd^{III} ions, and Gd^{III} and Zn^{II} ions are bridged by bidentate α-methylacrylato groups. The complex crystallizes in space group $P\bar{1}$ with $Z = 1$, $a = 13.4504(6)$, $b = 14.9697(5)$, $c = 16.4374(5)$ Å, $\alpha = 64.212(3)$, $\beta = 89.727(2)$, $\gamma = 86.241(1)°$. The structure was refined to $R = 0.0303$ for 8925 observed reflections. The temperature dependence of the magnetic susceptibility of the complex shows that a weak intramolecular ferromagnetic interaction exists as well as an intermolecular antiferromagnetic interaction.

Keywords: Gadolinium; Zinc; Heteronuclear; Magnetic properties; Crystal structure

INTRODUCTION

There has been increasing interest in the properties and stereochemistry of heteronuclear complexes comprising transition metal and lanthanide ions, primarily owing to electronic, electrochemical and magnetic properties arising from metal–metal interaction [1–4], and their mimicking of active centres of some metalloenzymes such as superoxide dismutase [5], cytochromic oxidase [6], hydrogenase [7], etc. Until now many polynuclear complexes containing both rare earth and transition metal ions, including Co [8], Ni [9], Cu [10], Fe [11], Mn [12] and Pd [13], have been synthesized and studied. In contrast, investigations of the Ln–Zn system, especially with respect to its magnetic properties, have rarely been reported [14]. The present investigation was undertaken to prepare the title complex ($[Gd_2Zn_2L_{10}(bipy)(H_2O)_2]_2$ (HL = α-methylacrylic acid, bipy = 4,4′-bipyridine)) and determine the structure for studying further magnetic properties of the complex and also as part of our studies of heteronuclear complexes of rare earth and transition metals bridged by α-unsaturated carboxyl groups.

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*Corresponding author. E-mail: weimwlu@mail.hz.zj.cn

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EXPERIMENTAL

GdL_3 was synthesized according to the literature [15]. All other chemicals were of reagent grade quality obtained from commercial sources and used without further purification. Elemental analyses were performed on a Cobra-Erba1110 instrument. IR spectra were recorded on a Nicolet 560 IR spectrophotometer. Magnetic data for the complex were measured using a Quantum Design model 6000 magnetometer over the temperature range 5–300 K at 10 kOe applied field.

Synthesis

$GdL_3 \cdot 2H_2O$ (897 mg, 2.0 mmol, $HL = CH_2C(CH_3)CO_2H$) and $Zn(NO_3)_2 \cdot 6H_2O$ (240 mg, 0.8 mmol) were dissolved in H_2O (20 cm^3) and adjusted to pH 4.1 with HL (0.1 M). An EtOH (5 cm^3) solution of 4,4′-bipy (60 mg, 0.4 mmol) was added to the mixed solution with stirring. After filtration, the filtrate was allowed to stand at room temperature and single crystals suitable for X-ray work were obtained after two weeks. Analysis: found: C, 40.42; H, 4.25; N, 1.95%; Calc. for $C_{100}H_{124}N_4O_{44}Gd_4Zn_4$: C, 40.35, H; 4.23; N; 1.88%. IR: ν_{as}(COO) 1557, ν_s (COO) 1429, ν (C=C) 1647 cm^{-1}.

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Crystal Structure Determination

A colourless, blocky crystal of $C_{100}H_{124}N_4O_{44}Gd_4Zn_4$ was mounted on a glass fibre. Data collection and processing were carried out on a Bruker SMART/CCD system. Cell refinement gave cell constants corresponding to a triclinic cell whose dimensions are given in Table I along with other experimental parameters. An empirical absorption correction was applied.

The structure was solved by direct methods [16]. All of the non-hydrogen atoms were treated anisotropically. Hydrogen atoms, with the exception of those of the water molecules, were included in idealized positions with isotropic thermal parameters set at 1.5 times for that of the tetrahedral carbon atoms to which they were attached, at 1.2 times for planar carbon. Full-matrix least-squares refinement [17] based on 8925 reflections with $I > 2.0\sigma(I)$ and 725 variable parameters converged smoothly (largest parameter shift in the final cycle was 0.004 times its e.s.d).

RESULTS AND DISCUSSION

Crystal Structure

Final atomic coordinates and equivalent isotropic thermal parameters for all non-H atoms are presented in Table II. Selected bond distances and angles are listed in Table III. Figure 1 shows an ORTEP diagram of one half of the molecular structure with the numbering scheme for the complex.

As shown in Fig. 1, the complex consists of a discrete octanuclear molecule, which possesses a symmetry centre between two gadolinium(III) ions. Links between metallic ions are made by two kinds of ligands. Gadolinium(III) ions are linked by two bridging carboxylato groups, zinc(II) and gadolinium(III) ions are bridged by three carboxylato groups and zinc(II) ions are linked by a 4,4′-bipy molecule. There are two different

TABLE I Crystallographic data for the complex

Chemical formula	$C_{100}H_{124}N_4O_{44}Gd_4Zn_4$
Molecular weight	2976.51
Crystal system	Triclinic
Space group	$P\bar{1}$
a (Å)	13.4504(6)
b (Å)	14.9697(5)
c (Å)	16.4374(5)
α (°)	64.212(3)
β (°)	89.727(2)
γ (°)	86.241(1)
V (Å^3)	2972.6(2)
Colour	Colourless
D_c (g cm^{-3})	1.663
Z	1
$F(000)$	1480
μ (mm^{-1})	3.074
hkl limits	−16, 15/−17, 17/−19, 19
θ range (°)	1.38 to 25.05
T (K)	293
Unique reflections	10281
Reflections with $I > 2.0\sigma(I)$	8925
Number of variables	725
R	0.0303
R_w	0.821
Maximum shift (Δ/σ)	0.004
Goodness-of-fit	1.198
Residual max in final difference map (e Å^{-3})	0.754 to −1.004

TABLE II Atomic coordinates and equivalent isotropic thermal parameters for non-H atoms

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
Gd1	0.503273(17)	0.362519(16)	0.144766(14)	0.03331(8)
Gd2	1.003888(17)	−0.298290(16)	1.356641(14)	0.03538(8)
Zn1	0.55134(4)	0.19934(4)	0.41478(3)	0.03997(14)
Zn2	0.87618(5)	−0.13791(5)	1.11861(4)	0.04334(15)
O1	0.4076(3)	0.2699(3)	0.2679(2)	0.0546(10)
O2	0.4108(3)	0.1783(3)	0.4143(2)	0.0534(9)
O3	0.6371(3)	0.2574(3)	0.2332(2)	0.0466(8)
O4	0.6296(3)	0.1237(3)	0.3636(2)	0.0491(9)
O5	0.5924(3)	0.3281(3)	0.3947(2)	0.0531(10)
O6	0.5454(3)	0.4233(3)	0.2528(2)	0.0577(10)
O7	0.4977(3)	0.1998(2)	0.1365(2)	0.0450(8)
O8	0.5705(3)	0.3196(3)	0.0272(2)	0.0489(9)
O9	0.3572(3)	0.3783(3)	0.0576(2)	0.0552(10)
O10	0.3933(3)	0.5158(3)	−0.0591(3)	0.0533(9)
O11	0.3994(3)	0.5140(3)	0.1290(3)	0.0550(11)
O12	0.9764(3)	−0.2199(3)	1.0904(2)	0.0633(11)
O13	0.9807(3)	−0.3302(3)	1.2323(2)	0.0529(9)
O14	0.9318(3)	−0.0236(3)	1.1253(2)	0.0544(9)
O15	1.0104(3)	−0.1329(3)	1.2489(2)	0.0539(9)
O16	0.7654(3)	−0.1853(3)	1.1983(2)	0.0532(9)
O17	0.8372(3)	−0.2389(3)	1.3335(2)	0.0556(10)
O18	1.0783(5)	−0.2233(4)	1.4416(3)	0.112(2)
O19	1.0007(4)	−0.3509(3)	1.5200(3)	0.0803(15)
O20	1.1285(3)	−0.4387(3)	1.4028(3)	0.0562(10)
O21	1.1750(3)	−0.2951(3)	1.3051(3)	0.0583(10)
O22	0.9147(3)	−0.4466(3)	1.4186(3)	0.0541(10)

(*continued*)

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TABLE II Continued

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
N1	0.5960(3)	0.1287(3)	0.5500(2)	0.0390(9)
N2	0.7984(3)	−0.0736(3)	0.9966(3)	0.0430(10)
C1	0.3665(4)	0.2201(4)	0.3386(3)	0.0404(11)
C2	0.2575(5)	0.2084(5)	0.3372(4)	0.0654(17)
C3	0.2066(6)	0.2554(7)	0.2569(5)	0.104(3)
C4	0.2135(6)	0.1425(9)	0.4219(5)	0.118(4)
C5	0.6599(4)	0.1677(4)	0.2841(3)	0.0387(11)
C6	0.7273(4)	0.1083(4)	0.2514(4)	0.0468(12)
C7	0.7634(5)	0.1506(6)	0.1687(4)	0.075(2)
C8	0.7498(7)	0.0040(5)	0.3128(6)	0.094(3)
C9	0.5907(4)	0.4081(4)	0.3234(3)	0.0421(11)
C10	0.6477(5)	0.4881(4)	0.3273(4)	0.0609(15)
C11	0.6702(8)	0.5638(6)	0.2489(7)	0.113(3)
C12	0.6755(8)	0.4790(7)	0.4148(7)	0.118(4)
C13	0.5422(4)	0.2314(4)	0.0633(3)	0.0433(12)
C14	0.5629(5)	0.1653(5)	0.0167(4)	0.0600(15)
C15	0.5767(9)	0.2079(7)	−0.0742(5)	0.121(4)
C16	0.5666(7)	0.0611(5)	0.0710(6)	0.090(2)
C17	0.3333(4)	0.4534(4)	−0.0137(3)	0.0409(11)
C18	0.2273(4)	0.4696(5)	−0.0439(4)	0.0577(15)
C19	0.1934(7)	0.5593(7)	−0.1131(6)	0.130(4)
C20	0.1598(6)	0.3949(7)	0.0019(6)	0.110(3)
C21	0.6712(4)	0.1659(4)	0.5742(3)	0.0526(14)
C22	0.7097(4)	0.1271(4)	0.6607(3)	0.0501(14)
C23	0.5582(4)	0.0488(4)	0.6140(3)	0.0431(12)
C24	0.5935(4)	0.0050(4)	0.7028(3)	0.0404(11)
C25	0.6712(3)	0.0451(4)	0.7282(3)	0.0366(10)
C26	0.7128(3)	0.0042(3)	0.8224(3)	0.0360(10)
C27	0.6997(4)	−0.0927(4)	0.8851(3)	0.0493(13)
C28	0.7431(4)	−0.1279(4)	0.9703(3)	0.0520(14)
C29	0.7677(4)	0.0608(4)	0.8508(3)	0.0401(11)
C30	0.8097(4)	0.0201(4)	0.9370(3)	0.0433(12)
C31	1.0107(4)	−0.2999(4)	1.1531(3)	0.0492(13)
C32	1.0891(5)	−0.3589(5)	1.1307(4)	0.0669(18)
C33	1.1082(8)	−0.4561(6)	1.1863(6)	0.114(3)
C34	1.1417(8)	−0.3107(9)	1.0494(6)	0.157(6)
C35	0.9854(4)	−0.0451(4)	1.1949(3)	0.0419(11)
C36	1.0209(4)	0.0381(4)	1.2118(4)	0.0475(12)
C37	1.0250(5)	0.1304(5)	1.1399(4)	0.0668(17)
C38	1.0490(6)	0.0170(5)	1.3021(4)	0.079(2)
C39	0.7623(4)	−0.2167(4)	1.2827(3)	0.0411(11)
C40	0.6614(4)	−0.2254(4)	1.3231(4)	0.0559(14)
C41	0.6551(7)	−0.2550(6)	1.4147(5)	0.092(2)
C42	0.5774(5)	−0.1992(6)	1.2643(6)	0.086(2)
C43	1.0487(4)	−0.2803(4)	1.5151(4)	0.0504(13)
C44	1.0757(6)	−0.2650(7)	1.5954(5)	0.081(2)
C45	1.0518(18)	−0.3397(12)	1.6782(7)	0.278(13)
C46	1.1173(9)	−0.1808(11)	1.5861(8)	0.173(7)
C47	1.1933(4)	−0.3868(4)	1.3516(4)	0.0487(13)
C48	1.2918(5)	−0.4360(5)	1.3456(4)	0.0622(16)
C49	1.3714(6)	−0.3738(7)	1.3106(6)	0.105(3)
C50	1.2987(6)	−0.5371(6)	1.3722(5)	0.092(3)

coordination geometries for the gadolinium ions in the complex. One gadolinium [Gd(1)] is coordinated by eight O atoms from one water molecule, five bridging bidentate and one chelating bidentate carboxylato groups. The other [Gd(2)] is also coordinated by eight O atoms, but from three bridging bidentate and two chelating

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TABLE III Selected bond distances (Å) and angles (°) for the complex

Bond distances			
Gd(1)–O(1)	2.333(3)	Gd(2)–O(19)	2.448(4)
Gd(1)–O(3)	2.344(3)	Gd(2)–O(20)	2.442(4)
Gd(1)–O(6)	2.405(3)	Gd(2)–O(21)	2.445(4)
Gd(1)–O(7)	2.503(3)	Gd(2)–O(22)	2.403(4)
Gd(1)–O(8)	2.439(3)	Zn(1)–O(2)	1.937(4)
Gd(1)–O(9)	2.374(4)	Zn(1)–O(4)	1.940(4)
Gd(1)–O(10)[a]	2.307(3)	Zn(1)–O(5)	1.927(4)
Gd(1)–O(11)	2.498(4)	Zn(1)–N(1)	2.075(4)
Gd(2)–O(13)	2.320(4)	Zn(2)–O(12)	1.952(4)
Gd(2)–O(15)	2.343(3)	Zn(2)–O(14)	1.958(4)
Gd(2)–O(17)	2.327(4)	Zn(2)–O(16)	1.936(4)
Gd(2)–O(18)	2.395(5)	Zn(2)–N(2)	2.062(4)
Bond angles			
O(1)–Gd(1)–O(3)	84.52(13)	O(13)–Gd(2)–O(22)	77.50(14)
O(1)–Gd(1)–O(6)	77.65(14)	O(15)–Gd(2)–O(17)	76.83(14)
O(1)–Gd(1)–O(7)	76.67(13)	O(15)–Gd(2)–O(18)	77.69(16)
O(1)–Gd(1)–O(8)	129.13(13)	O(15)–Gd(2)–O(19)	124.15(14)
O(1)–Gd(1)–O(9)	84.58(13)	O(15)–Gd(2)–O(20)	130.54(13)
O(1)–Gd(1)–O(10)[a]	157.52(14)	O(15)–Gd(2)–O(21)	77.65(14)
O(1)–Gd(1)–O(11)	87.95(14)	O(15)–Gd(2)–O(22)	148.44(14)
O(3)–Gd(1)–O(6)	73.55(13)	O(17)–Gd(2)–O(18)	106.1(2)
O(3)–Gd(1)–O(7)	72.41(12)	O(17)–Gd(2)–O(19)	92.37(18)
O(3)–Gd(1)–O(8)	84.30(12)	O(17)–Gd(2)–O(20)	149.13(15)
O(3)–Gd(1)–O(9)	146.75(14)	O(17)–Gd(2)–O(21)	151.75(16)
O(3)–Gd(1)–O(10)[a]	92.39(13)	O(17)–Gd(2)–O(22)	76.29(16)
O(3)–Gd(1)–O(11)	139.47(14)	O(18)–Gd(2)–O(19)	52.71(17)
O(6)–Gd(1)–O(7)	138.81(12)	O(18)–Gd(2)–O(20)	94.0(2)
O(6)–Gd(1)–O(8)	143.76(14)	O(18)–Gd(2)–O(21)	79.6(2)
O(6)–Gd(1)–O(9)	133.84(14)	O(18)–Gd(2)–O(22)	126.14(17)
O(6)–Gd(1)–O(10)[a]	80.11(14)	O(19)–Gd(2)–O(20)	82.24(18)
O(6)–Gd(1)–O(11)	65.94(13)	O(19)–Gd(2)–O(21)	112.16(19)
O(7)–Gd(1)–O(8)	52.65(11)	O(19)–Gd(2)–O(22)	73.58(17)
O(7)–Gd(1)–O(9)	74.53(13)	O(20)–Gd(2)–O(21)	53.18(14)
O(7)–Gd(1)–O(10)[a]	123.59(13)	O(20)–Gd(2)–O(22)	73.27(14)
O(7)–Gd(1)–O(11)	143.55(14)	O(21)–Gd(2)–O(22)	123.15(15)
O(8)–Gd(1)–O(9)	78.54(14)	O(2)–Zn(1)–O(4)	111.55(17)
O(8)–Gd(1)–O(10)[a]	72.39(13)	O(2)–Zn(1)–O(5)	119.85(18)
O(8)–Gd(1)–O(11)	129.18(12)	O(2)–Zn(1)–N(1)	104.72(15)
O(9)–Gd(1)–O(10)[a]	108.92(13)	O(4)–Zn(1)–O(5)	118.43(17)
O(9)–Gd(1)–O(11)	71.23(15)	O(4)–Zn(1)–N(1)	102.32(15)
O(10)[a]–Gd(1)–O(11)	79.97(14)	O(5)–Zn(1)–N(1)	95.45(15)
O(13)–Gd(2)–O(15)	84.46(13)	O(12)–Zn(2)–O(14)	112.40(19)
O(13)–Gd(2)–O(17)	85.57(14)	O(12)–Zn(2)–O(16)	126.20(19)
O(13)–Gd(2)–O(18)	155.55(17)	O(12)–Zn(2)–N(2)	98.94(16)
O(13)–Gd(2)–O(19)	150.50(14)	O(14)–Zn(2)–O(16)	112.33(17)
O(13)–Gd(2)–O(20)	83.79(14)	O(14)–Zn(2)–N(2)	102.62(16)
O(13)–Gd(2)–O(21)	79.51(14)	O(16)–Zn(2)–N(2)	98.98(16)

[a] Symmetry code: $-x+1$, $-y+1$, $-z$.

bidentate carboxylato groups and a water molecule. The coordination sphere around each gadolinium(III) ion is irregular. Each zinc(II) ion is four-coordinated by three O atoms from three bridging carboxylato groups and one N atom of a 4,4′-bipy group. The coordination polyhedron is a distorted tetrahedron.

As shown in Table III, there are three different distances, Gd–O$_{\text{chelating}}$, Gd–O$_{\text{bridging}}$ and Gd–O$_{\text{water}}$, between gadolinium and oxygen atoms in the title complex. Average bond lengths are 2.445, 2.344 and 2.451 Å, respectively. It is expected that the

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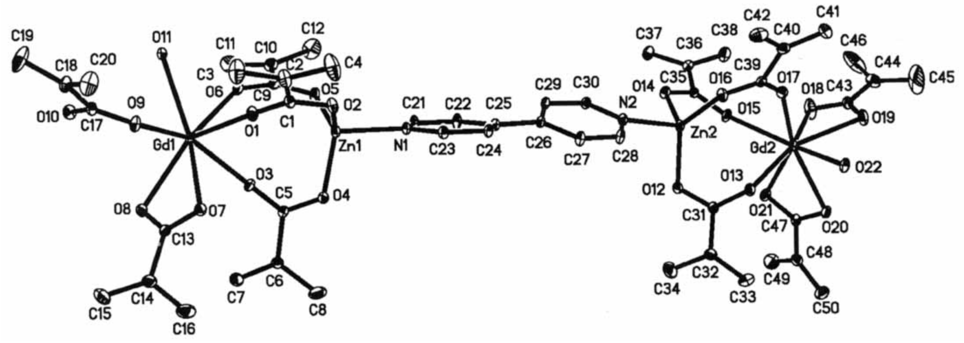

FIGURE 1 Half of the molecular structure and the atom numbering scheme for the complex with ellipsoids drawn at the 20% probability level. H atoms have been omitted for clarity.

Gd–O$_{\text{chelating}}$ distance is longer than that of Gd–O$_{\text{bridging}}$ because of ring strain in the four-membered rings. Six Zn–O bond distances are nearly the same from 1.927 to 1.958 Å and the average bond length is 1.942 Å. Zn–N bond lengths are similar, with an average value of 2.069 Å. Zn–O and Zn–N distances in the complex are shorter than those in [$NdZn_2L_6(NO_3)(phen)_2$], in which around Zn(II) ion has a trigonal bipyramidal configuration [14]. The neighboring Gd1···Zn1, Gd2···Zn2 and Gd1···Gd1A (symmetry code: $-x+1$, $-y+1$, $-z$) separations are 4.058, 3.921 and 4.754 Å, respectively, which exceed the sum of corresponding radii [18]. It is noteworthy that the Gd1···Gd1A separation in the complex is significantly longer than that (4.0456 Å) in [$La(CH_2C(Me)COO)_3(phen)(HL)]_2$ [19], in which there are four bridging carboxylato groups between the two La atoms.

IR Spectra

The carboxyl groups give rise to very strong IR absorptions [20], which can be used to distinguish between the different coordination modes of the ligands (ionic, monodentate or bidentate) [21]. The carboxyl group stretching vibration was observed at 1557 cm^{-1} [ν_{asym}(COO)] and 1429 cm^{-1} [ν_{sym}(COO)] in the complex. Separation (128 cm^{-1}) between ν_{asym}(COO) and ν_{sym}(COO) is indicative of bidentate coordination because it is smaller than the 146 cm^{-1} value for the corresponding sodium salt. However, spectroscopic techniques could not correctly identify bridging bidentate and chelating bidentate ligands.

Magnetic Properties

The temperature dependence of magnetic susceptibilities in the 5–300 K range under a 10 kOe applied DC field was measured. Molar magnetic susceptibilities were corrected for diamagnetic contributions and a plot of $\chi_m T$ and $1/\chi_m$ *vs* T is presented in Fig. 2 with χ_m being the molar magnetic susceptibility and T the temperature. The $\chi_m T$ value is 33.00 emu K mol^{-1} at 300K and increases very slowly to a maximum of 33.49 emu K mol^{-1} at 29K, then decreases to 31.02 emu K mol^{-1} at 5K. Contributions to the magnetic susceptibility ultimately come from Gd(III) ions as Zn(II) ions are diamagnetic. The effective magnetic moment μ_{eff} per Gd(III) ion at 300K is 8.12 BM, which is slightly larger than the calculated value of 7.94 BM.

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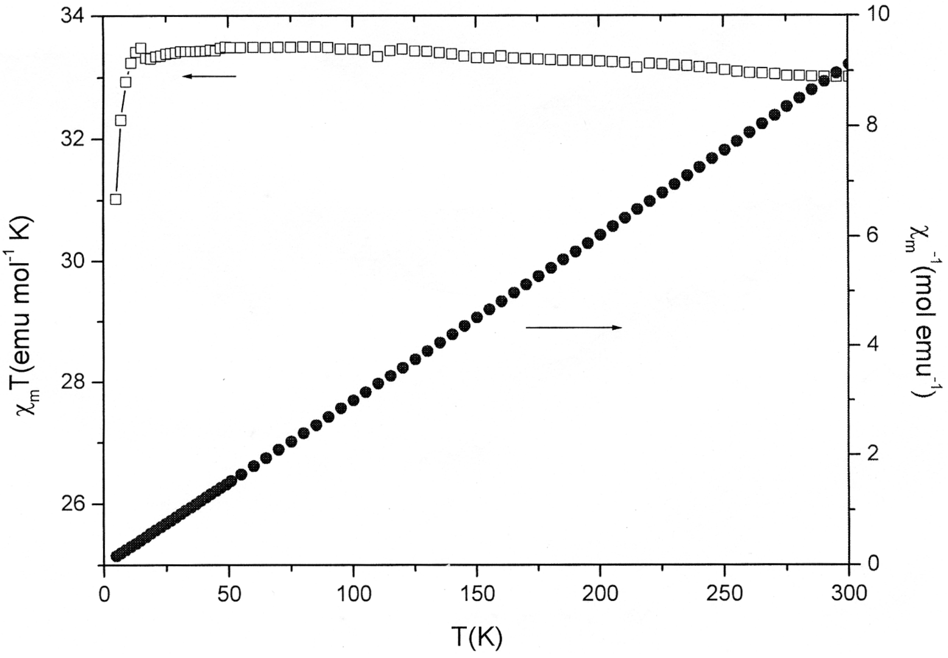

FIGURE 2 Plots of $\chi_m T$ and $1/\chi_m$ *vs* T for the complex.

Plots of $1/\chi_m$ *vs* T basically follow the Curie–Weiss law with the Curie constant $C = 33.05\,\mathrm{emu\,K\,mol^{-1}}$ and the Weiss constant $\theta = 0.65\mathrm{K}$. Magnetic behavior of the complex hints at a weak intramolecular ferromagnetic interaction and an intermolecular antiferromagnetic interaction. However, zero field AC measurements did not give any peaks for either real χ' or imaginary χ''. The value of $\chi_m T$ rapidly decreases upon further cooling below 29K, and this could be associated with the intermolecular antiferromagnetic interactions (Gd2···Gd2 = 5.832 Å) and zero field splitting effects, or a zero field splitting effect only.

Supplementary material

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Center, CCDC No. 191286. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk; http://www.ccdc.cam.ac.uk).

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