

Poly[*diaqua-μ*<sub>4</sub>-benzene-1,4-dicarboxylato-*di-μ*<sub>2</sub>-benzene-1,4-dicarboxylato-bis(*N,N'*-dimethylformamide)digadolinium(III)]

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## Key indicators

Single-crystal X-ray study  
*T* = 292 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.017  
*wR* factor = 0.042  
Data-to-parameter ratio = 16.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

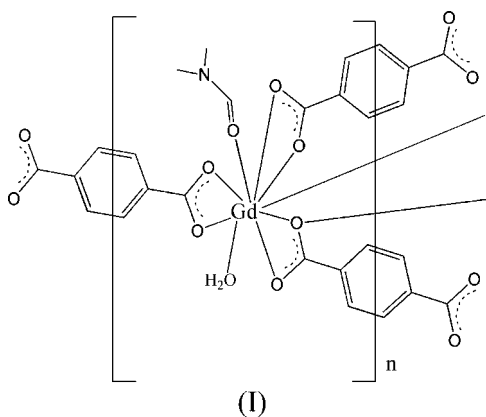
In the title compound,  $[\text{Gd}_2(\text{C}_8\text{H}_4\text{O}_4)_3(\text{C}_3\text{H}_7\text{NO})_2(\text{H}_2\text{O})_2]_n$ , the central  $\text{Gd}^{\text{III}}$  atom is nine-coordinated by seven O atoms from benzene-1,4-dicarboxylate (1,4-BDC) ligands, one dimethylformamide and one water molecule in a distorted tricapped trigonal-prism coordination. The 1,4-BDC ligands link the  $\text{Gd}^{\text{III}}$  atoms, forming a three-dimensional structure. All aromatic rings are located on centres of inversion. The water molecule forms hydrogen bonds to carboxylate groups.

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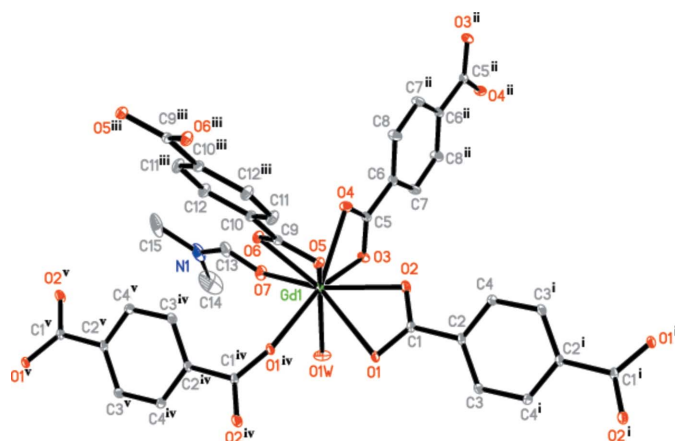
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## Comment

There has been tremendous interest in the syntheses and crystal structures of open-framework materials due to their potential applications in catalysis, separation and ion exchange processes (Eddaoudi *et al.*, 2001). As functional metal centres, lanthanide metals have received intense attention because of their physical and chemical properties. So far, extensive work has been carried out using carboxylate-containing ligands, such as benzene-1,2,4,5-tetracarboxylic acid, trimesic acid, benzene-1,4-dicarboxylic acid and naphthalene-2,6-dicarboxylic acid (Liu *et al.*, 2004). Benzene-1,4-dicarboxylic acid (1,4- $\text{H}_2\text{BDC}$ ) seems to be a promising organic linker because two carboxyl groups are able to establish bridges between several metal centres through various coordination modes and the conjugation with the aromatic ring allows it to become a rigid linker. Compared with transition metals, the analogous lanthanide complexes containing 1,4-BDC are still undeveloped, though some lanthanide coordination polymers have been reported in recent years (Guo *et al.*, 2006; Wan *et al.*, 2003; Pan *et al.*, 2001; Deluzet *et al.*, 2003). We report here the crystal structure of the title compound, (I), based on the 1,4-BDC ligand.



In (I), each  $\text{Gd}^{\text{III}}$  atom is coordinated by nine O atoms, *viz.* seven from the carboxylate groups of 1,4-BDC ligands, one from a coordinated dimethylformamide molecule and one



**Figure 1**  
View of the local coordination of the Gd<sup>III</sup> atom with the atomic numbering scheme. Displacement ellipsoids are drawn at the 25% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)  $-x, -y, 1 - z$ ; (ii)  $1 - x, -y, 2 - z$ ; (iii)  $-1 - x, 1 - y, 2 - z$ .]

from a coordinated water molecule, resulting in a distorted tricapped trigonal prism. The Gd–O distances range from 2.3729 (19) to 2.7175 (18) Å.

## Experimental

A mixture of GdCl<sub>3</sub>·6H<sub>2</sub>O (1 mmol) and 1,4-H<sub>2</sub>BDC (10 mmol) was dissolved in *N,N'*-dimethylformamide (10 ml) and H<sub>2</sub>O (2 ml) at room temperature. Two drops of triethylenetetramine were added, and then 6 M HNO<sub>3</sub> until the mixture became clear. The mixture in a 50 ml beaker was left undisturbed at 328 K for 7 d, giving colourless crystals of (I).

### Crystal data

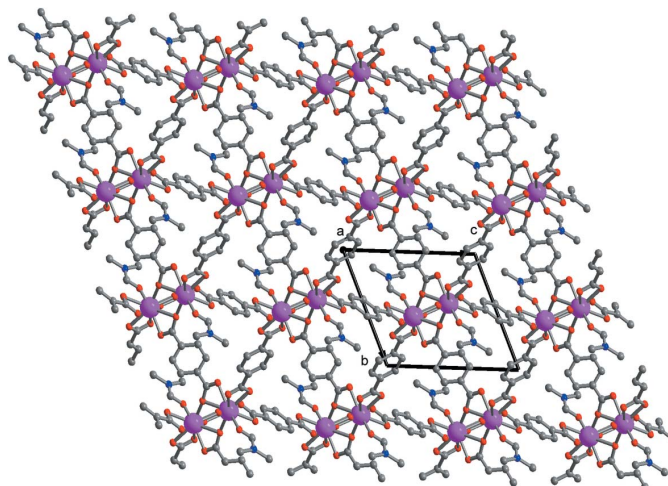
[Gd <sub>2</sub> (C <sub>8</sub> H <sub>4</sub> O <sub>4</sub> ) <sub>3</sub> (C <sub>3</sub> H <sub>7</sub> NO) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	$V = 839.1 (4) \text{ \AA}^3$
$M_r = 989.06$	$Z = 1$
Triclinic, <i>P1</i>	$D_x = 1.957 \text{ Mg m}^{-3}$
$a = 8.6066 (17) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.156 (2) \text{ \AA}$	$\mu = 4.00 \text{ mm}^{-1}$
$c = 11.161 (2) \text{ \AA}$	$T = 292 (2) \text{ K}$
$\alpha = 65.26 (3)^\circ$	Block, colourless
$\beta = 71.76 (3)^\circ$	$0.33 \times 0.31 \times 0.29 \text{ mm}$
$\gamma = 78.68 (3)^\circ$	

### Data collection

Rigaku R-AXIS RAPID diffractometer	8319 measured reflections
$\omega$ scans	3806 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	3626 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.253, T_{\max} = 0.316$	$R_{\text{int}} = 0.016$
	$\theta_{\text{max}} = 27.5^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.021P)^2 + 0.6587P]$
$R[F^2 > 2\sigma(F^2)] = 0.017$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.042$	$(\Delta/\sigma)_{\text{max}} = 0.003$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
3806 reflections	$\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$
232 parameters	
H atoms treated by a mixture of independent and constrained refinement	



**Figure 2**  
Packing diagram of (I); H atoms have been omitted for clarity.

**Table 1**

Selected geometric parameters (Å, °).

O1–Gd1	2.7175 (18)	O4–Gd1	2.4189 (19)
O2–Gd1	2.4343 (18)	O5–Gd1	2.4703 (19)
O1W–Gd1	2.404 (2)	O6–Gd1	2.4493 (19)
O3–Gd1	2.5143 (19)	O7–Gd1	2.3729 (19)
O7–Gd1–O1W	76.41 (8)	O6–Gd1–O5	53.04 (6)
O7–Gd1–O4	86.94 (8)	O7–Gd1–O3	76.20 (7)
O1W–Gd1–O4	131.44 (7)	O1W–Gd1–O3	78.70 (7)
O7–Gd1–O2	148.78 (7)	O4–Gd1–O3	52.93 (7)
O1W–Gd1–O2	97.10 (9)	O2–Gd1–O3	72.58 (7)
O4–Gd1–O2	74.52 (7)	O6–Gd1–O3	120.70 (6)
O7–Gd1–O6	73.86 (7)	O5–Gd1–O3	132.12 (6)
O1W–Gd1–O6	138.23 (8)	O7–Gd1–O1	147.14 (7)
O4–Gd1–O6	75.39 (7)	O1W–Gd1–O1	73.51 (7)
O2–Gd1–O6	123.21 (7)	O4–Gd1–O1	123.21 (6)
O7–Gd1–O5	126.74 (7)	O2–Gd1–O1	49.90 (6)
O1W–Gd1–O5	141.71 (7)	O6–Gd1–O1	122.76 (6)
O4–Gd1–O5	84.01 (7)	O5–Gd1–O1	74.09 (6)
O2–Gd1–O5	76.82 (7)	O3–Gd1–O1	110.02 (6)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W–HW11...O3 <sup>i</sup>	0.73 (3)	2.10 (3)	2.832 (3)	173 (3)
O1W–HW12...O5 <sup>ii</sup>	0.72 (3)	2.01 (3)	2.717 (3)	169 (3)

Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x, -y + 1, -z + 1$ .

All H atoms on C atoms were positioned geometrically and refined as riding, with C–H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms of the water molecule were located in a difference Fourier map and their coordinates were refined, while their  $U_{\text{iso}}$  values were set at 0.025 Å<sup>2</sup>.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL*.

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