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# Poly[bis($\mu_4$-1,4-benzenedicarboxylato)-($\mu_6$-succinato)digadolinium(III)]

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**Key indicators**

Single-crystal X-ray study
$T$ = 291 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.017
$wR$ factor = 0.044
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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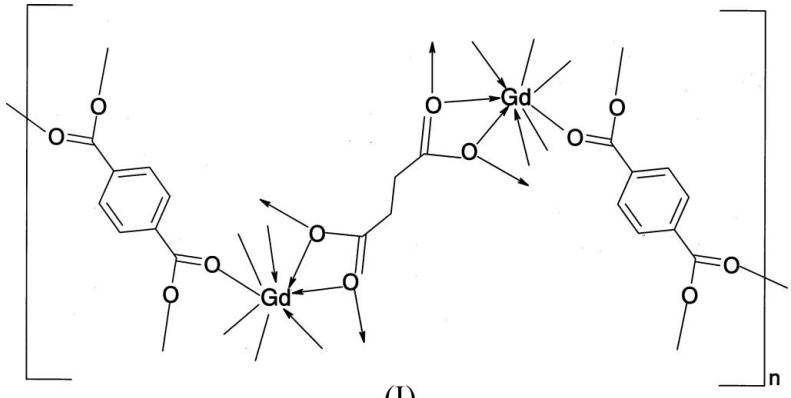
A new three-dimensional coordination polymer with the formula $[Gd_2(C_8H_4O_4)_2(C_4H_4O_4)]_n$ has been synthesized by hydrothermal synthesis. The coordination polyhedron around each Gd atom is a distorted square antiprism; the antiprisms are bridged into a three-dimensional network by the 1,4-benzenedicarboxylate and succinate ligands. The succinate ion is located on a centre of inversion.

## Comment

Variable coordination numbers (6–12) and geometries are observed in lanthanide complexes. Thus, the design of molecular architectures with predetermined structures is difficult (Drew, 1977; Reineke *et al.*, 1999). The rigid or semirigid polycarboxylate receptors may help to control the coordination sphere according to the lock-and-key and induced-fit concepts (Piguet & Bünzli, 1999). We have chosen the rigid aromatic 1,4-benzenedicarboxylate (BDC) and the saturated aliphatic succinate as ligands, to synthesize a ternary lanthanide coordination polymer with an open framework, $[Gd_2(C_8H_4O_4)_2(C_4H_4O_4)]_n$ (I).




(I)

As illustrated in Fig. 1, the $Gd^{3+}$ ion is coordinated in a distorted square antiprismatic geometry by four O atoms from four BDC and four from three succinate ions. The Gd—O bond distances range from 2.2723 (16) to 2.5654 (16) Å. In this structure, the succinate ligand is located on a centre of symmetry. Two carboxylate O atoms chelate one Gd atom and each O atom bridges another Gd atom with a Gd···Gd separation of 4.106 (2) Å. In this mode, the Gd atoms are bridged into one-dimensional infinite GdO chains along the [010] direction. A two-dimensional polymeric sheet is formed *via* bridging succinate ligands. The two-dimensional sheets are parallel to the *ab* plane and are bridged into a three-dimensional framework by BDC ligands. Is is noteworthy that one of

the carboxylate groups of the BDC ligand bridges two adjacent Gd atoms in the same chain (O3 and O4), while the other carboxylate group (O1 and O2) bridges two Gd atoms from neighbouring chains.

## Experimental

A mixture of $GdCl_3·6H_2O$ (1.00 mmol, 0.37 g), 1,4-benzenedicarboxylic acid (0.55 mmol, 0.09 g), succinic acid (0.51 mmol, 0.06 g), NaOH (2.00 mmol, 0.08 g) and $H_2O$ (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 443 K for 48 h. The colourless column-like crystals were filtered and washed with water and acetone (yield: 55%, based on Gd).

*Crystal data*

$[Gd_2(C_8H_4O_4)(C_4H_4O_4)]$
$M_r$ = 758.80
Orthorhombic, *Pbca*
$a$ = 13.9094 (9) Å
$b$ = 6.8497 (5) Å
$c$ = 21.8148 (14) Å
$V$ = 2078.4 (2) Å$^3$
$Z$ = 4
$D_x$ = 2.425 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 128 reflections
$\theta$ = 3.3–26.7°
$\mu$ = 6.40 mm$^{-1}$
$T$ = 291 (2) K
Plate cut from column, colourless
0.17 × 0.15 × 0.08 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.344, $T_{max}$ = 0.605
11172 measured reflections
2491 independent reflections
2303 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 28.0°
$h = -12 \rightarrow 18$
$k = -9 \rightarrow 9$
$l = -28 \rightarrow 27$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.044
$S$ = 1.06
2491 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 2.0093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.83 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.29 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00185 (9)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Gd—O2$^{i}$ | 2.2723 (16) | Gd—O5$^{iv}$ | 2.4341 (19) |
| Gd—O1 | 2.3305 (15) | Gd—O6$^{v}$ | 2.4837 (17) |
| Gd—O3$^{ii}$ | 2.3394 (16) | Gd—O5 | 2.5148 (16) |
| Gd—O4$^{iii}$ | 2.3560 (16) | Gd—O6 | 2.5654 (16) |

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+\frac{3}{2}, -y+2, z-\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

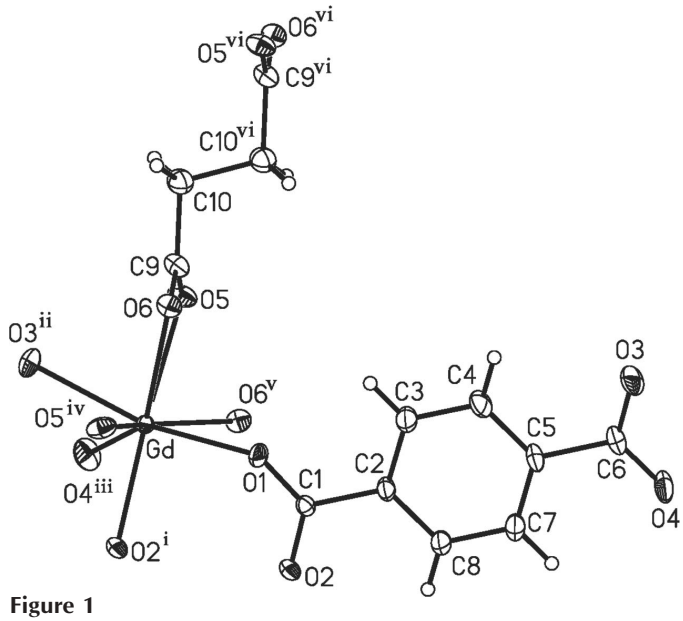



**Figure 1**
The coordination environment of the Gd atom, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 45% probability level. [Symmetry codes: (i) $1-x, 2-y, 1-z$; (ii) $\frac{3}{2}-x, 2-y, z-\frac{1}{2}$; (iii) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (iv) $\frac{3}{2}-x, \frac{1}{2}+y, z$; (v) $\frac{3}{2}-x, y-\frac{1}{2}, z$; (vi) $2-x, 2-y, 1-z$.]

H atoms were included at calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The deepest hole is located 0.84 Å from atom Gd.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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