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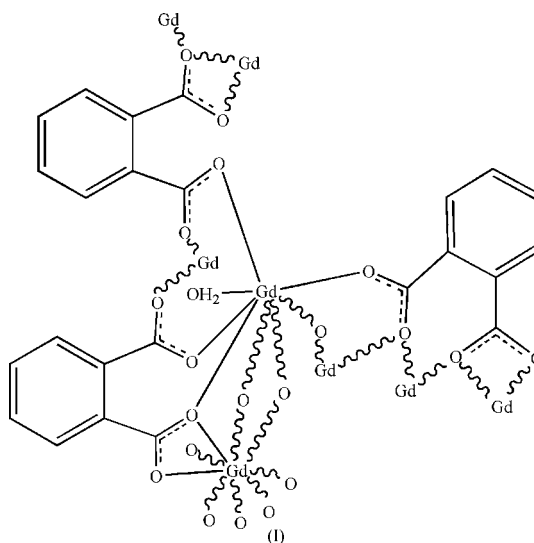
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Key indicators

Single-crystal X-ray study
 $T = 290\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.043
 wR factor = 0.111
Data-to-parameter ratio = 14.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[aquabis(μ_4 -benzene-1,2-dicarboxylato)-
(μ_3 -benzene-1,2-dicarboxylato)digadolinium(III)]The title compound, $[\text{Gd}_2(\text{C}_8\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})]_n$, is a two-dimensional coordination polymer. The Gd atoms are eight- and nine-coordinated. This compound is isostructural with its dysprosium analog.Received 22 March 2006
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Comment

The title compound, $[\text{Gd}_2(\text{bdc})_3(\text{H}_2\text{O})]_n$ (bdc is benzene-1,2-dicarboxylate), (I), possesses a two-dimensional infinite structure. Its asymmetric unit contains two gadolinium ions (Fig. 1). Atom Gd1 is eight-coordinated by O atoms (Table 1), seven of which come from carboxylate groups of five bdc anions and the other from a water molecule. Atom Gd2 is nine-coordinated by O atoms from the carboxylate groups of six bdc anions. One of the Gd2—O bonds is significantly longer than the others. It is noteworthy that in the complex all the H_2bdc molecules are completely deprotonated and the O atoms coordinate to the Gd^{III} ions in three different modes, which results in a two-dimensional layer-like structure (Fig. 2). The compound is isostructural with its dysprosium analog (Song *et al.*, 2004). The distribution of C—O bond lengths in (I) suggests that the negative charges of some of the carboxylate groups are completely delocalized, while others are essentially localized. The water molecule participates in two O—H...O links (Table 2).



Experimental

A mixture of Gd_2O_3 (0.091 g, 0.25 mmol), L-glutamic acid (0.147 g, 1 mmol), H_2bdc (0.166 g, 1 mmol) and H_2O (10 ml) was sealed in a 20 ml Teflon-lined stainless steel vessel and heated to 443 K for 72 h. After the vessel had been cooled slowly to room temperature, colorless rod-shaped crystals of (I) were obtained.

Crystal data

[Gd₂(C₈H₄O₄)₃(H₂O)]
M_r = 824.85
 Monoclinic, *P*2₁/*c*
a = 7.9786 (5) Å
b = 26.4255 (15) Å
c = 11.6508 (8) Å
 β = 107.048 (3)°
V = 2348.5 (3) Å³

Z = 4
D_x = 2.333 Mg m⁻³
 Mo *K*α radiation
 μ = 5.67 mm⁻¹
T = 290 (2) K
 Rod, colorless
 0.60 × 0.11 × 0.10 mm

Data collection

Rigaku Mercury CCD
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.125, *T_{max}* = 0.567

17823 measured reflections
 5352 independent reflections
 4551 reflections with *I* > 2σ(*I*)
R_{int} = 0.056
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.043
wR(*F*²) = 0.111
 S = 1.06
 5352 reflections
 358 parameters

H atoms treated by a mixture of
 independent and constrained
 refinement
 $w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 2.33 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -2.45 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Gd1—O1	2.293 (4)	Gd2—O3	2.679 (4)
Gd1—O11 ⁱ	2.306 (4)	Gd2—O10	2.885 (5)
Gd1—O6 ⁱⁱ	2.348 (4)	C1—O1	1.263 (7)
Gd1—O9	2.397 (4)	C1—O2	1.251 (7)
Gd1—O7	2.403 (4)	C8—O3	1.270 (7)
Gd1—O13	2.410 (4)	C8—O4	1.265 (7)
Gd1—O5	2.474 (4)	C9—O5	1.273 (7)
Gd1—O3	2.521 (4)	C9—O6	1.243 (7)
Gd2—O12 ⁱⁱⁱ	2.244 (4)	C16—O7	1.289 (7)
Gd2—O2 ^{iv}	2.282 (4)	C16—O8	1.232 (7)
Gd2—O5	2.418 (4)	C17—O9	1.299 (7)
Gd2—O4	2.430 (4)	C17—O10	1.236 (8)
Gd2—O9	2.434 (4)	C24—O11	1.242 (7)
Gd2—O8 ⁱⁱⁱ	2.453 (4)	C24—O12	1.248 (7)
Gd2—O7 ⁱⁱⁱ	2.525 (4)		
Gd1—O3—Gd2	92.80 (13)	Gd1—O9—Gd2	102.49 (15)
Gd2—O5—Gd1	100.72 (15)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O13—H13B...O3 ⁱⁱ	0.84 (5)	2.06 (6)	2.893 (6)	171 (8)
O13—H13C...O10 ^v	0.84 (5)	1.85 (6)	2.677 (6)	170 (6)

Symmetry codes: (ii) *x*, −*y* + $\frac{3}{2}$, *z* + $\frac{1}{2}$; (v) *x* − 1, *y*, *z*.

C-bound H atoms were positioned geometrically in idealized positions (C—H = 0.93 Å) and refined as riding with *U*_{iso}(H) = 1.2*U*_{eq}(C). The aqua H atoms were located in a difference map and refined with the restraints O—H = 0.84 (1) Å and H...H = 1.4 (1) Å and with *U*_{iso}(H) = 1.5*U*_{eq}(O). The highest peak and deepest hole in the difference map are located 1.49 and 0.81 Å, respectively, from atoms O5 and Gd2.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve

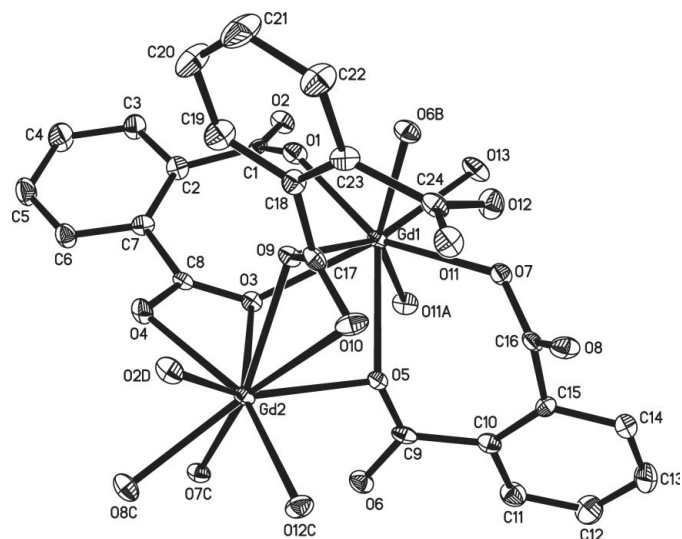


Figure 1
 The coordination environment of the Gd atoms in (I), shown with 50% probability displacement ellipsoids. [Symmetry codes: (A) *x* − 1, −*y* + $\frac{3}{2}$, *z* − $\frac{1}{2}$; (B) *x*, −*y* + $\frac{3}{2}$, *z* + $\frac{1}{2}$; (C) *x*, −*y* + $\frac{3}{2}$, *z* − $\frac{1}{2}$; (D) *x* + 1, *y*, *z*.]

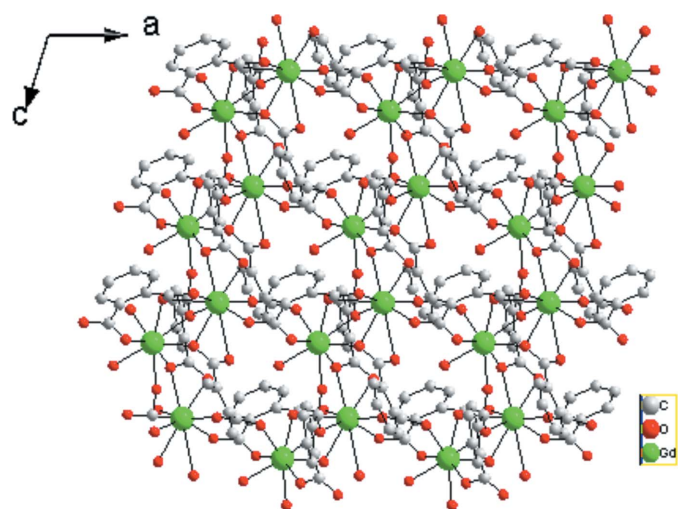


Figure 2
 The two-dimensional structure of (I). All H atoms have been omitted for clarity.

structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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