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**Key indicators**

Single-crystal X-ray study  
 T = 294 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
 R factor = 0.023  
 wR factor = 0.052  
 Data-to-parameter ratio = 14.4

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

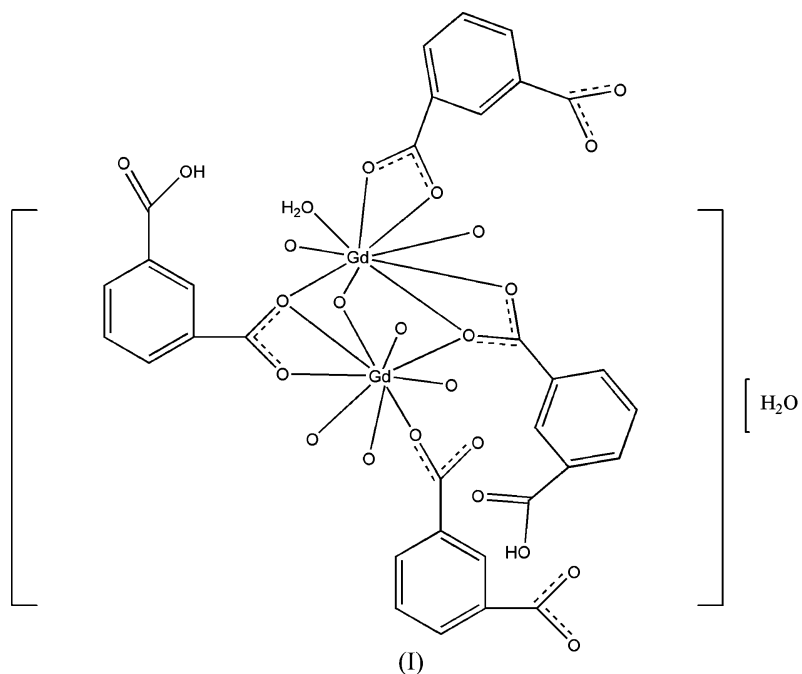
**Poly[[aquabis( $\mu$ -benzene-1,3-dicarboxylato)-  
 bis( $\mu$ -3-carboxybenzoato)digadolinium(III)]  
 monohydrate]**

In the title compound,  $[\text{Gd}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_8\text{H}_5\text{O}_4)_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$ , the  $\text{Gd}^{\text{III}}$  ions are nine-coordinated and linked by carboxylate O bridges, giving rise to right- and left-handed inorganic helical chains. The crystal structure is stabilized by intra- and intermolecular O–H...O hydrogen bonds, linking the chains into a three-dimensional framework.

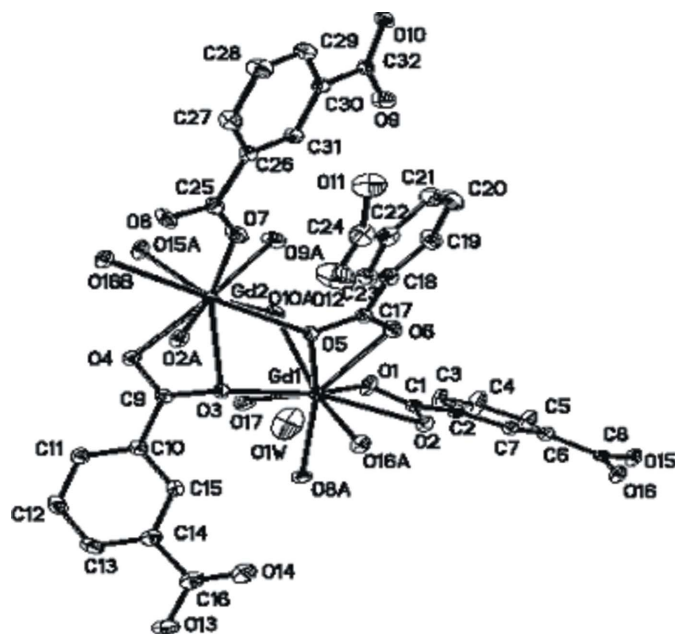
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**Comment**

The construction of metal–organic frameworks (MOFs) is of current interest in the field of crystal engineering and supramolecular chemistry, stemming not only from their potential applications as functional materials (Leininger *et al.*, 2000) but also their intriguing variety of architectures and molecular topologies (Bradshaw *et al.*, 2005). However, MOFs, based on right- and left-handed inorganic helical chains, constructed from  $\pi$ – $\pi$  stacking effects and hydrogen bonds, are less developed. Here we report a new three-dimensional microporous MOF based on right- and left-handed inorganic helical chains constructed from hydrogen bonds.



The overall structure of the title compound, (I), is of a three-dimensional hydrogen-bonded framework, based on a two-dimensional layer structure constructed of helical chains. In the asymmetric unit there are two independent  $\text{Gd}^{\text{III}}$  ions, two ip (completely deprotonated *m*-phthalic acid) ligands, two Hip (singly deprotonated *m*-phthalic acid) ligands, one coor-



**Figure 1**  
A drawing of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

minated water molecule and one uncoordinated water molecule. Gd1 is nine-coordinated by O atoms of ip and Hip ligands and a water molecule in a tricapped trigonal–prismatic geometry. Gd2 also adopts a GdO<sub>9</sub> tricapped trigonal–prismatic geometry, which is defined by O atoms of ip and Hip ligands (Fig. 1).

The Gd–O bond lengths span the range 2.358 (2)–2.666 (2) Å. The ip ligands show pentadentate and hexadentate coordination modes, while the Hip ligands exhibit a tridentate coordinated mode with one carboxyl group undeprotonated; this is confirmed by IR analysis (the bands at 1727 and 1690 cm<sup>-1</sup> are derived from the undeprotonated carboxyl groups, while the deprotonated carboxyl groups are characterized by the bands at 1606 and 1484 cm<sup>-1</sup>; Kakihana *et al.*, 1987).

The Gd<sup>III</sup> ions are further linked by ip and Hip ligands, giving a two-dimensional layer structure (Fig. 2) in which the nine-coordinated Gd1 and Gd2 atoms are bridged, with Gd···Gd distances of 3.8278 (7) and 4.111 (1) Å, respectively, by carboxylate O atoms from ip and Hip ligands, leading to the left- and right-handed helical chains.

To the best of our knowledge, this type of inorganic helical chain linked by carboxylate O atoms is rare. Another structural feature of (I) is the three-dimensional hydrogen-bonded framework with a one-dimensional trigonal channel (6 Å) along [001] filled with water molecules. The uncoordinated water molecules are involved in typical hydrogen bonds (Table 2).

## Experimental

An aqueous mixture of Gd<sub>2</sub>O<sub>3</sub> (181 mg, 0.5 mmol) and H<sub>2</sub>ip (166 mg, 1.0 mmol) (10 ml) was placed in a Teflon reactor (23 ml), heated for

5 d, and then cooled to room temperature. Colourless crystals were obtained in 68% yield based on Gd.

### Crystal data

[Gd<sub>2</sub>(C<sub>8</sub>H<sub>4</sub>O<sub>4</sub>)<sub>2</sub>(C<sub>8</sub>H<sub>5</sub>O<sub>4</sub>)<sub>2</sub>·(H<sub>2</sub>O)]·H<sub>2</sub>O  
*M<sub>r</sub>* = 1009.00  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.438 (2) Å  
*b* = 13.811 (3) Å  
*c* = 21.254 (4) Å  
 $\beta$  = 95.60 (3)°

*V* = 3049.3 (11) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 2.198 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 4.40 mm<sup>-1</sup>  
*T* = 294 (2) K  
 Block, colourless  
 0.34 × 0.16 × 0.11 mm

### Data collection

Rigaku R-AXIS RAPID-S IP area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.303, *T<sub>max</sub>* = 0.617

28964 measured reflections  
 6991 independent reflections  
 6489 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.042  
 $\theta_{\max}$  = 27.5°

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.023  
*wR* (*F*<sup>2</sup>) = 0.052  
*S* = 1.05  
 6991 reflections  
 487 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.4415P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.006$   
 $\Delta\rho_{\max} = 0.76 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.96 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Gd1–O8 <sup>i</sup>	2.358 (2)	Gd2–O7	2.271 (2)
Gd1–O1	2.371 (2)	Gd2–O2 <sup>iii</sup>	2.397 (2)
Gd1–O3	2.374 (2)	Gd2–O9 <sup>ii</sup>	2.413 (2)
Gd1–O10 <sup>ii</sup>	2.470 (2)	Gd2–O5	2.418 (2)
Gd1–O17	2.472 (2)	Gd2–O15 <sup>iv</sup>	2.438 (2)
Gd1–O16 <sup>iii</sup>	2.492 (2)	Gd2–O4	2.507 (2)
Gd1–O6	2.563 (2)	Gd2–O3	2.513 (2)
Gd1–O5	2.580 (2)	Gd2–O16 <sup>iv</sup>	2.602 (2)
Gd1–O2	2.666 (2)	Gd2–O10 <sup>ii</sup>	2.669 (2)
Gd1–Gd2	3.8278 (7)		
O8 <sup>i</sup> –Gd1–O1	87.80 (8)	O7–Gd2–O2 <sup>iii</sup>	78.92 (8)
O8 <sup>i</sup> –Gd1–O3	90.76 (7)	O7–Gd2–O9 <sup>ii</sup>	73.25 (8)
O1–Gd1–O3	146.95 (7)	O2 <sup>iii</sup> –Gd2–O9 <sup>ii</sup>	148.69 (8)
O8 <sup>i</sup> –Gd1–O10 <sup>ii</sup>	138.51 (7)	O7–Gd2–O5	85.68 (8)

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

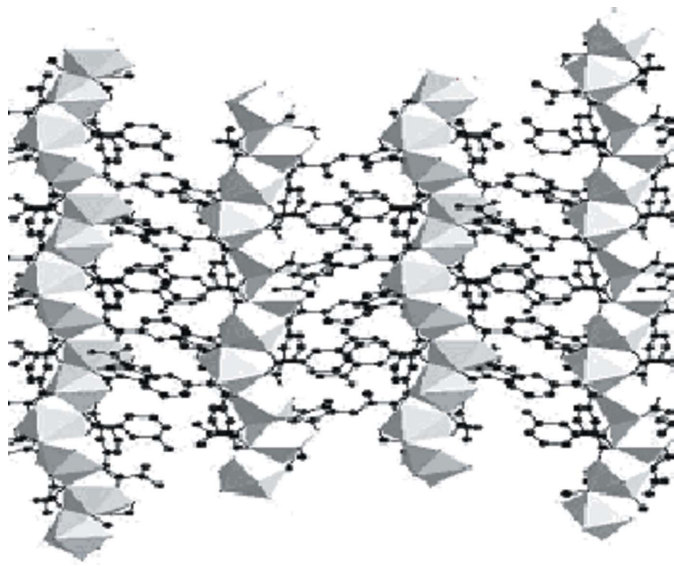
**Table 2**

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>
O17–H17B···O1W	0.85 (4)	1.92 (4)	2.769 (5)	173 (5)
O1W–H1WB···O12 <sup>i</sup>	0.85 (7)	2.11 (4)	2.918 (5)	158 (10)
O1W–H1WA···O4 <sup>v</sup>	0.85 (1)	2.21 (3)	2.989 (4)	152 (6)

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

Water H atoms were located in difference maps and refined isotropically with distance restraints O–H = 0.85 (1) and H···H = 1.45 (1) Å] and *U<sub>iso</sub>*(H) = 0.055 (15)–0.16 (4) Å<sup>2</sup>. The remaining H atoms were positioned geometrically, with O–H = 0.82 Å and C–H = 0.93 Å, and constrained to ride on their parent atoms, with *U<sub>iso</sub>*(H)



**Figure 2**  
A view of the two-dimensional structure of (I), based on the left- and right-handed helical chains.

$= xU_{eq}(C,O)$ , where  $x = 1.2$  for aromatic H and  $x = 1.5$  for all other H atoms.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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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