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# *catena*-Poly[[[diaqua[3-(pyridin-4-yl)-benzoato-$\kappa^2O,O'$]gadolinium(III)]-bis[$\mu$-3-(pyridin-4-yl)benzoato-$\kappa^2O:O'$]] monohydrate]

**Dong-Ying Li* and Guo-Ting Li**

Department of Environmental and Municipal Engineering, North China University of Water Conservancy and Electric Power, Zhengzhou 450011, People's Republic of China
Correspondence e-mail: lidongying@ncwu.edu.cn

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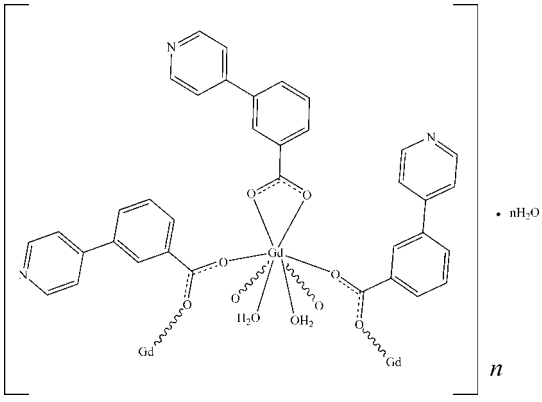
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.025; $wR$ factor = 0.061; data-to-parameter ratio = 12.4.

In the title coordination polymer, $\{[Gd(C_{12}H_8NO_2)_3(H_2O)_2]\cdot H_2O\}_n$, the $Gd^{III}$ ion is ligated by one bidentate carboxylate group, four monodentate bridging carboxylate O atoms and two water molecules. The resulting $GdO_8$ polyhedron approximates to a square antiprism. The bridging ligands link the metal ions into a [100] chain, with each pair of adjacent metal ions being bridged by two ligands. Inter-chain O—H···O and O—H···N hydrogen bonds help to establish the packing.

## Related literature

For metal-organic frameworks containing aromatic carboxylic ligands, see: Li *et al.* (2010). For lanthanide metal-organic frameworks based on aromatic carboxylic ligands, see: Zhang *et al.* (2010). For transition metal coordination complexes of 3-pyridin-4-ylbenzoate, see: Wu *et al.* (2011).




## Experimental

### Crystal data

$[Gd(C_{12}H_8NO_2)_3(H_2O)_2]\cdot H_2O$
$M_r$ = 805.88
Triclinic, $P\overline{1}$
$a$ = 9.7252 (5) Å
$b$ = 13.9535 (6) Å
$c$ = 14.0829 (8) Å
$\alpha$ = 118.019 (5)°
$\beta$ = 104.240 (5)°
$\gamma$ = 90.089 (4)°
$V$ = 1619.84 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.11 mm$^{-1}$
$T$ = 293 K
0.35 × 0.21 × 0.18 mm

### Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.970, $T_{max}$ = 1.000
12338 measured reflections
5702 independent reflections
4844 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.061
$S$ = 1.05
5702 reflections
460 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.85 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.66 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Gd1—O5$^{i}$ | 2.290 (2) | Gd1—O8 | 2.443 (2) |
| Gd1—O4$^{ii}$ | 2.295 (2) | Gd1—O7 | 2.447 (2) |
| Gd1—O3 | 2.395 (2) | Gd1—O2 | 2.468 (2) |
| Gd1—O6 | 2.405 (2) | Gd1—O1 | 2.532 (2) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O7—H7$A$···O1$^{i}$ | 0.71 (3) | 2.12 (3) | 2.826 (3) | 173 (4) |
| O7—H7$B$···N1$^{iii}$ | 0.89 (4) | 1.89 (4) | 2.772 (4) | 173 (3) |
| O8—H8$B$···O2$^{ii}$ | 0.75 (3) | 2.05 (3) | 2.793 (3) | 173 (4) |
| O8—H8$A$···N3$^{iv}$ | 0.84 (4) | 1.95 (4) | 2.789 (4) | 175 (3) |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Natural Science Foundation of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6834).

## References

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Zhang, L. J., Xu, D. H., Zhou, Y. S. & Jiang, F. (2010). *New J. Chem.* **34**, 2470–2478.

# supplementary materials

*Acta Cryst.* (2012). E**68**, m928–m929 [doi:10.1107/S1600536812026153]

## *catena*-Poly[[[diaqua[3-(pyridin-4-yl)benzoato-$\kappa^2O,O'$]gadolinium(III)]-bis-[$\mu$-3-(pyridin-4-yl)benzoato-$\kappa^2O$:$O'$]] monohydrate]

**Dong-Ying Li and Guo-Ting Li**

### Comment

Aromatic carboxylic ligands have been widely used to construct metal-organic frameworks (MOFs) with novel structures and unique properties (Li *et al.*, 2010). Especially, lanthanide MOFs of aromatic carboxylic ligands have largely drawn current attention (Zhang, *et al.*, 2010) owing to their potential applications in medical imaging, sensors and electro-optical devices. 3-Pyridin-4-ylbenzoic acid (HL) which possess a pyridyl group and a benzoic acid group is a typical unsymmetrical spacer, and up to now only a serial of its transition metal coordination complexes was synthesized and characterized (Wu, *et al.*, 2011). Herein we report the synthesis and structure of a gadolinium(III) complex of deprotonated 3-pyridin-4-ylbenzoic acid (HL), namely, $[Gd(L)_3(H_2O)_2]_n$ (1).n($H_2O$).

In (1), the Gd atom is in an eight-coordinate environment of $O_8$ ligated by six carboxylato O atoms from five ligands *L* and two O atoms from water molecules (Fig. 1). The Gd—O bonds fall in the normal range from 2.290 (2) to 2.532 (2) Å. In (1), deprotonated ligands *L* act as bidentate ligands, and display two coordinating modes, namely, chelating and bridging coordination models of carboxyl groups without the nitrogen atoms of the pyridyl groups taking part in the coordination. Complex (1) is a two-stranded polymeric chain builted from two *L* simultaneously bridging adjacent two Gd side by side and two *L* chelating them up and down with the separations of the adjacent metal Gd ions bridged by the carboxylato O3 and O4 of one *L*, and by the carboxylato O5 and O6 of the other *L* being 4.833 and 4.895 Å, respectively (Fig. 2). Apart from intrachain O—H···O hydrogen bonds, the chains of complex (1) are connected by interchain O—H···N hydrogen bonds between the coordinated water molecules (as donors) and the uncoordinated pyridyl groups of *L* (as acceptors), leading to the formation of a three-dimensional network structure with uncoordinated water molecules residing in the accessible void.

### Experimental

A mixture of $Gd(NO_3)_3$ (0.045 g, 0.1 mmol), HL (0.060 g, 0.3 mmol), NaOH (0.012 0.3 mmol) and deionized water (10 ml) was sealed into a 25 ml Teflon-lined stainless autoclave. The autoclave was heated at 180 °C for four days. As cooled to room temperature gradually, colourless block crystals of (I) were obtained in 37% yield (based on Gd). Selected IR ($cm^{-1}$, KBr pellet): 3440(*s*), 1611(*m*), 1545(*m*), 1436(*s*), 1396(*s*), 1384(*s*), 1282(*w*), 1173(*s*), 1131(*s*), 766(*m*), 719(*m*), 655(*m*).

### Refinement

The H atoms of water were located from difference Fourier maps and included in the final refinement by using geometrical restrains, while the other hydrogen atom positions were generated geometrically and these H atoms were allowed to ride on their parent atoms.

### Computing details

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

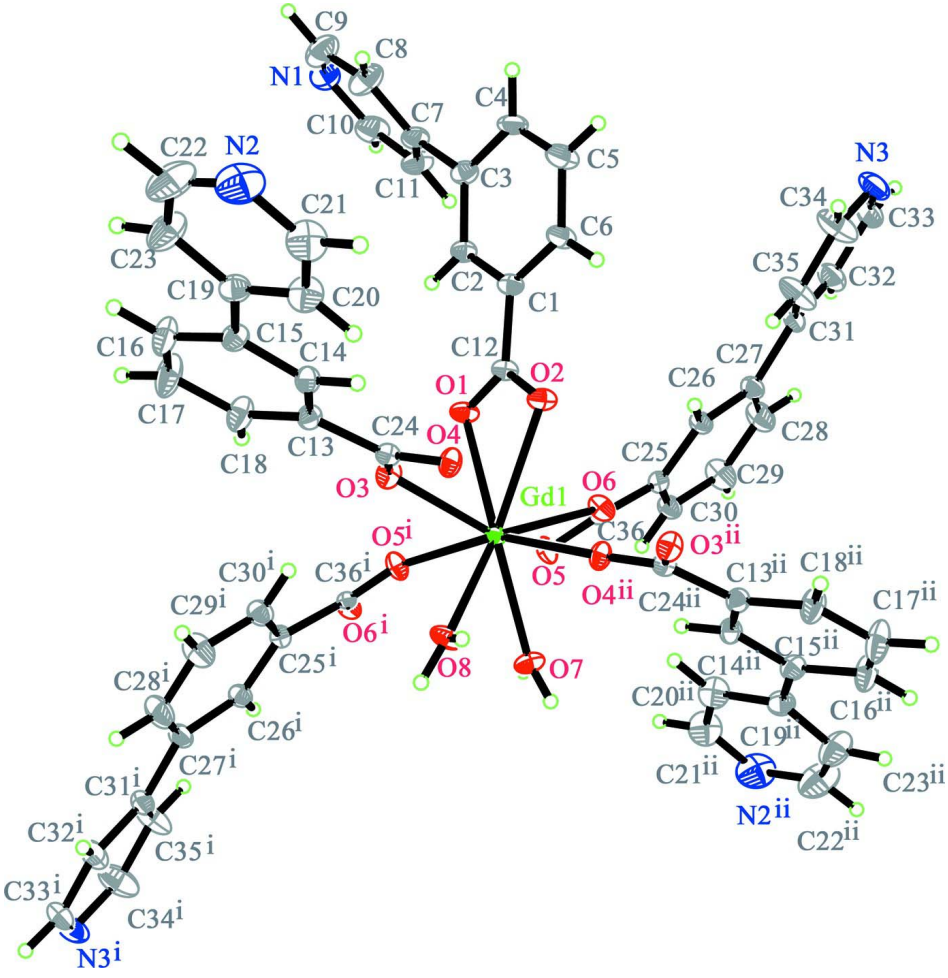


**Figure 1**

Coordination environment of the Gd atom in (1). Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) -*x*, -*y*, -*z*; (ii) -*x* + 1, -*y*, -*z*.

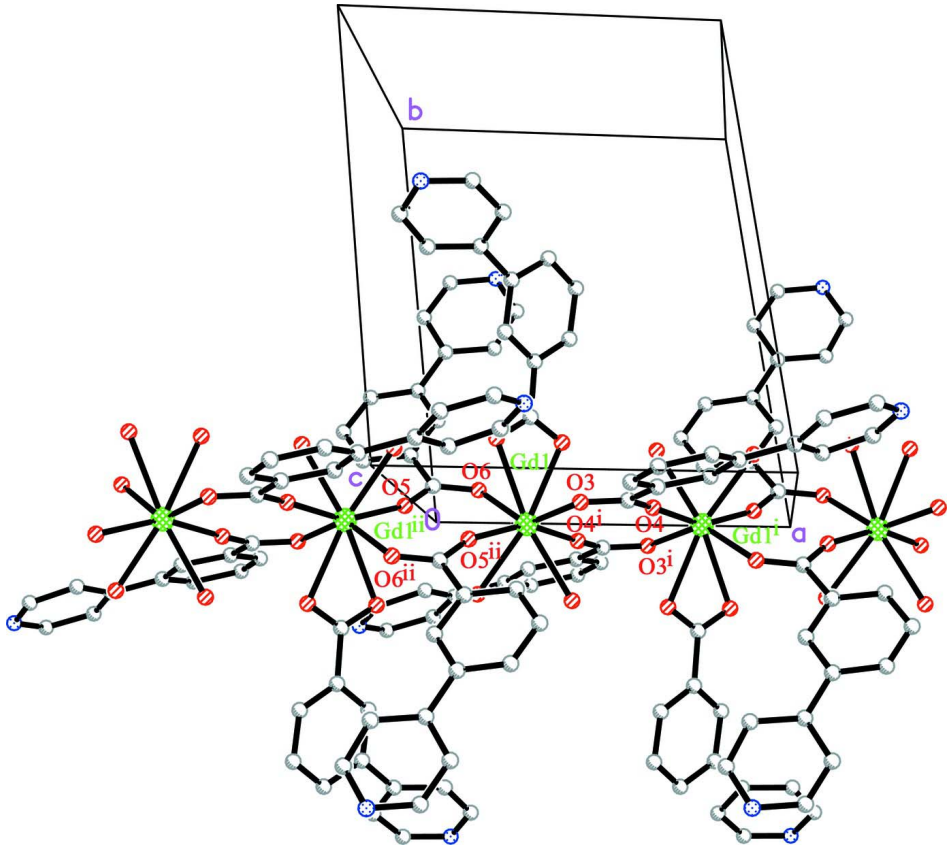


**Figure 2**

View of infinite two-stranded chain bridged by *L* in (1). Symmetry code: (i) -*x*, -*y*, -*z*; (ii) -*x* + 1, -*y*, -*z*.

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*Crystal data*

$[Gd(C_{12}H_8NO_2)_3(H_2O)_2]\cdot H_2O$
$M_r$ = 805.88
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.7252 (5) Å
$b$ = 13.9535 (6) Å
$c$ = 14.0829 (8) Å
$\alpha$ = 118.019 (5)°
$\beta$ = 104.240 (5)°
$\gamma$ = 90.089 (4)°
$V$ = 1619.84 (14) Å$^3$
$Z$ = 2
$F(000)$ = 806
$D_x$ = 1.652 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 8413 reflections
$\theta$ = 2.9–26.3°
$\mu$ = 2.11 mm$^{-1}$
$T$ = 293 K
Block, colourless
0.35 × 0.21 × 0.18 mm

*Data collection*

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.970, $T_{max}$ = 1.000
12338 measured reflections
5702 independent reflections
4844 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.023
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.9°
$h$ = −11→11
$k$ = −16→16
$l$ = −16→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.061
$S$ = 1.05
5702 reflections
460 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 0.5641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.85 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.66 e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Gd1 | 0.252518 (15) | −0.002199 (12) | 0.002647 (12) | 0.01875 (6) |
| O1 | 0.2075 (2) | 0.17870 (18) | 0.15035 (19) | 0.0298 (5) |
| O2 | 0.3835 (2) | 0.18197 (17) | 0.07980 (19) | 0.0290 (5) |
| O3 | 0.4213 (2) | 0.03112 (19) | 0.17419 (19) | 0.0307 (5) |
| O4 | 0.6183 (2) | 0.02697 (19) | 0.12145 (18) | 0.0284 (5) |
| O5 | −0.0958 (2) | 0.04584 (19) | −0.0786 (2) | 0.0310 (5) |
| O6 | 0.1155 (2) | 0.08726 (18) | −0.0915 (2) | 0.0295 (5) |
| O7 | 0.0774 (2) | −0.1512 (2) | −0.1568 (2) | 0.0312 (6) |
| O8 | 0.3516 (3) | −0.17299 (19) | −0.0343 (2) | 0.0333 (6) |
| O9 | 0.3749 (6) | 0.2281 (5) | −0.1164 (5) | 0.1291 (19) |
| N1 | 0.1269 (4) | 0.6874 (3) | 0.6483 (3) | 0.0487 (9) |
| N2 | 1.3290 (4) | 0.2014 (3) | 0.5396 (4) | 0.0674 (11) |
| N3 | 0.2287 (4) | 0.6204 (3) | −0.0892 (3) | 0.0560 (10) |
| C1 | 0.3436 (3) | 0.3525 (3) | 0.2204 (3) | 0.0268 (7) |
| C2 | 0.2774 (3) | 0.4068 (3) | 0.3048 (3) | 0.0285 (7) |
| H2 | 0.2038 | 0.3674 | 0.3114 | 0.034* |
| C3 | 0.3178 (4) | 0.5181 (3) | 0.3797 (3) | 0.0320 (8) |
| C4 | 0.4266 (4) | 0.5753 (3) | 0.3694 (3) | 0.0384 (9) |
| H4 | 0.4578 | 0.6507 | 0.4217 | 0.046* |
| C5 | 0.4884 (4) | 0.5218 (3) | 0.2832 (3) | 0.0441 (10) |
| H5 | 0.5597 | 0.5613 | 0.2746 | 0.053* |
| C6 | 0.4478 (4) | 0.4114 (3) | 0.2092 (3) | 0.0349 (8) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.4914 | 0.3755 | 0.1503 | 0.042* |
| C7 | 0.2509 (4) | 0.5773 (3) | 0.4722 (3) | 0.0343 (8) |
| C8 | 0.3328 (5) | 0.6354 (3) | 0.5820 (3) | 0.0514 (11) |
| H8 | 0.4341 | 0.6393 | 0.5998 | 0.062* |
| C9 | 0.2673 (5) | 0.6879 (4) | 0.6658 (4) | 0.0609 (13) |
| H9 | 0.3263 | 0.7268 | 0.7408 | 0.073* |
| C10 | 0.0485 (5) | 0.6331 (3) | 0.5419 (4) | 0.0509 (11) |
| H10 | −0.0522 | 0.6332 | 0.5267 | 0.061* |
| C11 | 0.1031 (4) | 0.5768 (3) | 0.4523 (3) | 0.0444 (10) |
| H11 | 0.0413 | 0.5384 | 0.3782 | 0.053* |
| C12 | 0.3088 (3) | 0.2315 (3) | 0.1464 (3) | 0.0246 (7) |
| C13 | 0.6422 (3) | 0.0531 (3) | 0.3047 (3) | 0.0264 (7) |
| C14 | 0.7906 (3) | 0.0751 (3) | 0.3354 (3) | 0.0276 (7) |
| H14 | 0.8363 | 0.0731 | 0.2823 | 0.033* |
| C15 | 0.8737 (3) | 0.0999 (3) | 0.4416 (3) | 0.0299 (8) |
| C16 | 0.8041 (4) | 0.0999 (4) | 0.5168 (3) | 0.0477 (11) |
| H16 | 0.8584 | 0.1169 | 0.5901 | 0.057* |
| C17 | 0.6570 (4) | 0.0754 (4) | 0.4861 (3) | 0.0563 (12) |
| H17 | 0.6113 | 0.0735 | 0.5377 | 0.068* |
| C18 | 0.5758 (4) | 0.0535 (3) | 0.3811 (3) | 0.0404 (9) |
| H18 | 0.4744 | 0.0387 | 0.3614 | 0.048* |
| C19 | 1.0316 (4) | 0.1321 (3) | 0.4756 (3) | 0.0341 (8) |
| C20 | 1.1051 (4) | 0.1240 (3) | 0.3992 (4) | 0.0446 (10) |
| H20 | 1.0552 | 0.0931 | 0.3220 | 0.053* |
| C21 | 1.2497 (4) | 0.1605 (4) | 0.4350 (4) | 0.0548 (11) |
| H21 | 1.2952 | 0.1559 | 0.3808 | 0.066* |
| C22 | 1.2615 (5) | 0.2065 (4) | 0.6113 (4) | 0.0720 (15) |
| H22 | 1.3162 | 0.2343 | 0.6871 | 0.086* |
| C23 | 1.1152 (4) | 0.1742 (4) | 0.5848 (4) | 0.0566 (12) |
| H23 | 1.0733 | 0.1812 | 0.6416 | 0.068* |
| C24 | 0.5544 (3) | 0.0352 (3) | 0.1922 (3) | 0.0236 (7) |
| C25 | −0.0766 (3) | 0.1751 (3) | −0.1399 (3) | 0.0234 (7) |
| C26 | 0.0122 (3) | 0.2600 (3) | −0.1274 (3) | 0.0268 (7) |
| H26 | 0.1128 | 0.2649 | −0.0993 | 0.032* |
| C27 | −0.0424 (4) | 0.3386 (3) | −0.1553 (3) | 0.0314 (8) |
| C28 | −0.1895 (4) | 0.3258 (3) | −0.2000 (4) | 0.0465 (10) |
| H28 | −0.2296 | 0.3774 | −0.2209 | 0.056* |
| C29 | −0.2787 (4) | 0.2405 (3) | −0.2148 (4) | 0.0463 (10) |
| H29 | −0.3789 | 0.2332 | −0.2466 | 0.056* |
| C30 | −0.2230 (4) | 0.1656 (3) | −0.1837 (3) | 0.0316 (8) |
| H30 | −0.2848 | 0.1077 | −0.1922 | 0.038* |
| C31 | 0.0522 (4) | 0.4346 (3) | −0.1337 (3) | 0.0349 (8) |
| C32 | −0.0024 (5) | 0.5242 (3) | −0.1383 (3) | 0.0491 (11) |
| H32 | −0.1030 | 0.5246 | −0.1565 | 0.059* |
| C33 | 0.0871 (6) | 0.6126 (3) | −0.1170 (4) | 0.0559 (12) |
| H33 | 0.0448 | 0.6718 | −0.1224 | 0.067* |
| C34 | 0.2818 (5) | 0.5352 (4) | −0.0836 (5) | 0.0685 (14) |
| H34 | 0.3830 | 0.5385 | −0.0628 | 0.082* |
| C35 | 0.2005 (5) | 0.4419 (3) | −0.1060 (4) | 0.0586 (13) |

| | | | | |
|---|---|---|---|---|
| H35 | 0.2459 | 0.3830 | −0.1024 | 0.070* |
| C36 | −0.0144 (3) | 0.0968 (2) | −0.1011 (2) | 0.0203 (7) |
| H7A | 0.004 (4) | −0.156 (3) | −0.158 (3) | 0.030* |
| H8A | 0.318 (4) | −0.235 (3) | −0.047 (3) | 0.030* |
| H7B | 0.088 (3) | −0.207 (3) | −0.219 (3) | 0.030* |
| H8B | 0.422 (4) | −0.181 (3) | −0.048 (3) | 0.030* |
| H9B | 0.450 (3) | 0.198 (3) | −0.132 (3) | 0.030* |
| H9A | 0.359 (4) | 0.189 (3) | −0.087 (3) | 0.030* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Gd1 | 0.01859 (9) | 0.01705 (9) | 0.02183 (9) | 0.00224 (6) | 0.00914 (6) | 0.00871 (7) |
| O1 | 0.0271 (12) | 0.0209 (12) | 0.0364 (14) | 0.0000 (10) | 0.0167 (11) | 0.0063 (11) |
| O2 | 0.0239 (12) | 0.0224 (12) | 0.0353 (14) | 0.0021 (10) | 0.0154 (11) | 0.0065 (11) |
| O3 | 0.0215 (12) | 0.0426 (15) | 0.0293 (13) | 0.0027 (10) | 0.0080 (10) | 0.0181 (12) |
| O4 | 0.0270 (12) | 0.0393 (14) | 0.0239 (12) | 0.0062 (10) | 0.0126 (10) | 0.0164 (11) |
| O5 | 0.0294 (13) | 0.0361 (14) | 0.0416 (15) | 0.0049 (11) | 0.0149 (11) | 0.0274 (13) |
| O6 | 0.0198 (12) | 0.0311 (14) | 0.0434 (15) | 0.0055 (10) | 0.0073 (11) | 0.0234 (12) |
| O7 | 0.0210 (13) | 0.0284 (14) | 0.0306 (14) | 0.0001 (11) | 0.0099 (12) | 0.0023 (11) |
| O8 | 0.0273 (14) | 0.0206 (13) | 0.0557 (17) | 0.0068 (11) | 0.0211 (13) | 0.0170 (13) |
| O9 | 0.155 (5) | 0.143 (5) | 0.166 (5) | 0.077 (4) | 0.082 (4) | 0.117 (4) |
| N1 | 0.067 (3) | 0.035 (2) | 0.044 (2) | 0.0145 (18) | 0.029 (2) | 0.0121 (17) |
| N2 | 0.037 (2) | 0.074 (3) | 0.074 (3) | −0.008 (2) | 0.010 (2) | 0.025 (2) |
| N3 | 0.078 (3) | 0.032 (2) | 0.068 (3) | −0.0022 (19) | 0.033 (2) | 0.0253 (19) |
| C1 | 0.0235 (17) | 0.0210 (18) | 0.0311 (19) | 0.0030 (14) | 0.0040 (15) | 0.0107 (15) |
| C2 | 0.0273 (18) | 0.0241 (18) | 0.0302 (19) | 0.0036 (14) | 0.0093 (15) | 0.0096 (16) |
| C3 | 0.0324 (19) | 0.0254 (19) | 0.032 (2) | 0.0078 (15) | 0.0069 (16) | 0.0101 (16) |
| C4 | 0.046 (2) | 0.0195 (19) | 0.037 (2) | −0.0030 (16) | 0.0090 (18) | 0.0049 (17) |
| C5 | 0.047 (2) | 0.028 (2) | 0.055 (3) | −0.0019 (17) | 0.022 (2) | 0.014 (2) |
| C6 | 0.037 (2) | 0.0244 (19) | 0.042 (2) | 0.0016 (16) | 0.0195 (18) | 0.0117 (17) |
| C7 | 0.043 (2) | 0.0203 (18) | 0.033 (2) | 0.0084 (16) | 0.0128 (17) | 0.0071 (16) |
| C8 | 0.052 (3) | 0.050 (3) | 0.036 (2) | 0.022 (2) | 0.012 (2) | 0.008 (2) |
| C9 | 0.081 (4) | 0.050 (3) | 0.035 (2) | 0.022 (3) | 0.013 (2) | 0.009 (2) |
| C10 | 0.053 (3) | 0.036 (2) | 0.058 (3) | 0.009 (2) | 0.029 (2) | 0.012 (2) |
| C11 | 0.045 (2) | 0.034 (2) | 0.039 (2) | −0.0008 (18) | 0.0153 (19) | 0.0045 (18) |
| C12 | 0.0183 (16) | 0.0211 (17) | 0.0310 (19) | 0.0031 (13) | 0.0070 (14) | 0.0098 (15) |
| C13 | 0.0256 (18) | 0.0285 (19) | 0.0255 (18) | 0.0029 (14) | 0.0093 (15) | 0.0124 (15) |
| C14 | 0.0267 (18) | 0.0315 (19) | 0.0283 (19) | 0.0052 (15) | 0.0116 (15) | 0.0156 (16) |
| C15 | 0.0251 (18) | 0.033 (2) | 0.0283 (19) | 0.0023 (15) | 0.0048 (15) | 0.0136 (16) |
| C16 | 0.040 (2) | 0.077 (3) | 0.032 (2) | −0.002 (2) | 0.0036 (18) | 0.033 (2) |
| C17 | 0.039 (2) | 0.103 (4) | 0.037 (2) | −0.003 (2) | 0.0124 (19) | 0.041 (3) |
| C18 | 0.0252 (19) | 0.067 (3) | 0.032 (2) | −0.0013 (18) | 0.0079 (16) | 0.026 (2) |
| C19 | 0.0296 (19) | 0.033 (2) | 0.036 (2) | 0.0032 (16) | 0.0070 (17) | 0.0143 (17) |
| C20 | 0.027 (2) | 0.055 (3) | 0.050 (3) | 0.0052 (18) | 0.0067 (18) | 0.026 (2) |
| C21 | 0.034 (2) | 0.067 (3) | 0.066 (3) | 0.006 (2) | 0.016 (2) | 0.034 (3) |
| C22 | 0.040 (3) | 0.086 (4) | 0.051 (3) | −0.009 (3) | −0.011 (2) | 0.014 (3) |
| C23 | 0.037 (2) | 0.079 (3) | 0.037 (2) | −0.004 (2) | 0.0046 (19) | 0.017 (2) |
| C24 | 0.0217 (17) | 0.0223 (17) | 0.0269 (18) | 0.0034 (13) | 0.0084 (14) | 0.0112 (15) |
| C25 | 0.0238 (17) | 0.0247 (18) | 0.0242 (17) | 0.0043 (14) | 0.0076 (14) | 0.0134 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C26 | 0.0243 (17) | 0.0266 (18) | 0.0304 (19) | 0.0049 (14) | 0.0065 (15) | 0.0151 (16) |
| C27 | 0.038 (2) | 0.0240 (19) | 0.036 (2) | 0.0067 (15) | 0.0121 (17) | 0.0170 (17) |
| C28 | 0.043 (2) | 0.045 (3) | 0.064 (3) | 0.0128 (19) | 0.008 (2) | 0.039 (2) |
| C29 | 0.025 (2) | 0.053 (3) | 0.069 (3) | 0.0071 (18) | 0.0040 (19) | 0.041 (2) |
| C30 | 0.0281 (19) | 0.032 (2) | 0.037 (2) | 0.0001 (15) | 0.0078 (16) | 0.0185 (17) |
| C31 | 0.050 (2) | 0.028 (2) | 0.035 (2) | 0.0037 (17) | 0.0189 (18) | 0.0182 (17) |
| C32 | 0.060 (3) | 0.037 (2) | 0.057 (3) | 0.003 (2) | 0.010 (2) | 0.031 (2) |
| C33 | 0.095 (4) | 0.031 (2) | 0.051 (3) | 0.007 (2) | 0.021 (3) | 0.027 (2) |
| C34 | 0.059 (3) | 0.048 (3) | 0.112 (4) | 0.001 (2) | 0.036 (3) | 0.044 (3) |
| C35 | 0.055 (3) | 0.041 (3) | 0.101 (4) | 0.010 (2) | 0.033 (3) | 0.046 (3) |
| C36 | 0.0264 (18) | 0.0155 (16) | 0.0164 (16) | −0.0001 (13) | 0.0068 (13) | 0.0054 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Gd1—O5$^{i}$ | 2.290 (2) | C9—H9 | 0.9500 |
| Gd1—O4$^{ii}$ | 2.295 (2) | C10—C11 | 1.375 (5) |
| Gd1—O3 | 2.395 (2) | C10—H10 | 0.9500 |
| Gd1—O6 | 2.405 (2) | C11—H11 | 0.9500 |
| Gd1—O8 | 2.443 (2) | C13—C18 | 1.382 (4) |
| Gd1—O7 | 2.447 (2) | C13—C14 | 1.389 (4) |
| Gd1—O2 | 2.468 (2) | C13—C24 | 1.505 (4) |
| Gd1—O1 | 2.532 (2) | C14—C15 | 1.388 (4) |
| O1—C12 | 1.257 (4) | C14—H14 | 0.9500 |
| O2—C12 | 1.270 (4) | C15—C16 | 1.390 (5) |
| O3—C24 | 1.252 (3) | C15—C19 | 1.491 (5) |
| O4—C24 | 1.261 (3) | C16—C17 | 1.381 (5) |
| O4—Gd1$^{ii}$ | 2.295 (2) | C16—H16 | 0.9500 |
| O5—C36 | 1.252 (3) | C17—C18 | 1.379 (5) |
| O5—Gd1$^{i}$ | 2.290 (2) | C17—H17 | 0.9500 |
| O6—C36 | 1.251 (3) | C18—H18 | 0.9500 |
| O7—H7A | 0.71 (3) | C19—C23 | 1.380 (5) |
| O7—H7B | 0.89 (4) | C19—C20 | 1.395 (5) |
| O8—H8A | 0.84 (4) | C20—C21 | 1.378 (5) |
| O8—H8B | 0.75 (3) | C20—H20 | 0.9500 |
| O9—H9B | 0.872 (10) | C21—H21 | 0.9500 |
| O9—H9A | 0.868 (10) | C22—C23 | 1.394 (6) |
| N1—C9 | 1.325 (5) | C22—H22 | 0.9500 |
| N1—C10 | 1.331 (5) | C23—H23 | 0.9500 |
| N2—C22 | 1.310 (6) | C25—C26 | 1.381 (4) |
| N2—C21 | 1.320 (6) | C25—C30 | 1.384 (4) |
| N3—C33 | 1.325 (6) | C25—C36 | 1.502 (4) |
| N3—C34 | 1.325 (5) | C26—C27 | 1.394 (4) |
| C1—C6 | 1.387 (4) | C26—H26 | 0.9500 |
| C1—C2 | 1.390 (4) | C27—C28 | 1.387 (5) |
| C1—C12 | 1.490 (4) | C27—C31 | 1.486 (5) |
| C2—C3 | 1.391 (5) | C28—C29 | 1.373 (5) |
| C2—H2 | 0.9500 | C28—H28 | 0.9500 |
| C3—C4 | 1.398 (5) | C29—C30 | 1.376 (5) |
| C3—C7 | 1.488 (5) | C29—H29 | 0.9500 |
| C4—C5 | 1.380 (5) | C30—H30 | 0.9500 |

| | | | |
|---|---|---|---|
| C4—H4 | 0.9500 | C31—C32 | 1.382 (5) |
| C5—C6 | 1.379 (5) | C31—C35 | 1.389 (5) |
| C5—H5 | 0.9500 | C32—C33 | 1.374 (6) |
| C6—H6 | 0.9500 | C32—H32 | 0.9500 |
| C7—C8 | 1.377 (5) | C33—H33 | 0.9500 |
| C7—C11 | 1.394 (5) | C34—C35 | 1.381 (5) |
| C8—C9 | 1.376 (5) | C34—H34 | 0.9500 |
| C8—H8 | 0.9500 | C35—H35 | 0.9500 |

| | | | |
|---|---|---|---|
| O5$^{i}$—Gd1—O4$^{ii}$ | 158.30 (9) | O1—C12—C1 | 120.5 (3) |
| O5$^{i}$—Gd1—O3 | 82.32 (8) | O2—C12—C1 | 119.3 (3) |
| O4$^{ii}$—Gd1—O3 | 106.79 (7) | O1—C12—Gd1 | 61.50 (16) |
| O5$^{i}$—Gd1—O6 | 103.62 (7) | O2—C12—Gd1 | 58.66 (16) |
| O4$^{ii}$—Gd1—O6 | 81.10 (7) | C1—C12—Gd1 | 177.8 (2) |
| O3—Gd1—O6 | 143.19 (8) | C18—C13—C14 | 119.1 (3) |
| O5$^{i}$—Gd1—O8 | 89.77 (8) | C18—C13—C24 | 120.3 (3) |
| O4$^{ii}$—Gd1—O8 | 74.67 (8) | C14—C13—C24 | 120.5 (3) |
| O3—Gd1—O8 | 73.33 (9) | C15—C14—C13 | 121.8 (3) |
| O6—Gd1—O8 | 141.74 (9) | C15—C14—H14 | 119.1 |
| O5$^{i}$—Gd1—O7 | 74.87 (9) | C13—C14—H14 | 119.1 |
| O4$^{ii}$—Gd1—O7 | 85.95 (8) | C14—C15—C16 | 117.9 (3) |
| O3—Gd1—O7 | 138.81 (8) | C14—C15—C19 | 120.8 (3) |
| O6—Gd1—O7 | 76.44 (8) | C16—C15—C19 | 121.2 (3) |
| O8—Gd1—O7 | 72.76 (9) | C17—C16—C15 | 120.7 (3) |
| O5$^{i}$—Gd1—O2 | 125.02 (8) | C17—C16—H16 | 119.6 |
| O4$^{ii}$—Gd1—O2 | 76.66 (8) | C15—C16—H16 | 119.6 |
| O3—Gd1—O2 | 74.77 (8) | C18—C17—C16 | 120.5 (4) |
| O6—Gd1—O2 | 72.28 (8) | C18—C17—H17 | 119.7 |
| O8—Gd1—O2 | 127.98 (8) | C16—C17—H17 | 119.7 |
| O7—Gd1—O2 | 146.07 (9) | C17—C18—C13 | 119.9 (3) |
| O5$^{i}$—Gd1—O1 | 74.17 (8) | C17—C18—H18 | 120.1 |
| O4$^{ii}$—Gd1—O1 | 126.86 (7) | C13—C18—H18 | 120.1 |
| O3—Gd1—O1 | 74.94 (8) | C23—C19—C20 | 115.1 (3) |
| O6—Gd1—O1 | 72.06 (8) | C23—C19—C15 | 122.8 (3) |
| O8—Gd1—O1 | 146.02 (9) | C20—C19—C15 | 122.1 (3) |
| O7—Gd1—O1 | 128.36 (7) | C21—C20—C19 | 120.4 (4) |
| O2—Gd1—O1 | 51.95 (7) | C21—C20—H20 | 119.8 |
| C12—O1—Gd1 | 92.62 (18) | C19—C20—H20 | 119.8 |
| C12—O2—Gd1 | 95.27 (18) | N2—C21—C20 | 124.2 (4) |
| C24—O3—Gd1 | 126.2 (2) | N2—C21—H21 | 117.9 |
| C24—O4—Gd1$^{ii}$ | 174.8 (2) | C20—C21—H21 | 117.9 |
| C36—O5—Gd1$^{i}$ | 163.6 (2) | N2—C22—C23 | 124.8 (4) |
| C36—O6—Gd1 | 125.31 (18) | N2—C22—H22 | 117.6 |
| Gd1—O7—H7A | 121 (3) | C23—C22—H22 | 117.6 |
| Gd1—O7—H7B | 131 (2) | C19—C23—C22 | 119.7 (4) |
| H7A—O7—H7B | 108 (4) | C19—C23—H23 | 120.2 |
| Gd1—O8—H8A | 134 (2) | C22—C23—H23 | 120.2 |
| Gd1—O8—H8B | 120 (3) | O3—C24—O4 | 123.2 (3) |
| H8A—O8—H8B | 105 (3) | O3—C24—C13 | 118.2 (3) |

| | | | |
|---|---|---|---|
| H9B—O9—H9A | 93 (3) | O4—C24—C13 | 118.5 (3) |
| C9—N1—C10 | 115.9 (4) | C26—C25—C30 | 119.6 (3) |
| C22—N2—C21 | 115.7 (4) | C26—C25—C36 | 119.8 (3) |
| C33—N3—C34 | 115.4 (4) | C30—C25—C36 | 120.5 (3) |
| C6—C1—C2 | 119.2 (3) | C25—C26—C27 | 121.5 (3) |
| C6—C1—C12 | 120.2 (3) | C25—C26—H26 | 119.3 |
| C2—C1—C12 | 120.6 (3) | C27—C26—H26 | 119.3 |
| C1—C2—C3 | 120.7 (3) | C28—C27—C26 | 117.2 (3) |
| C1—C2—H2 | 119.6 | C28—C27—C31 | 121.4 (3) |
| C3—C2—H2 | 119.6 | C26—C27—C31 | 121.4 (3) |
| C2—C3—C4 | 119.2 (3) | C29—C28—C27 | 121.9 (3) |
| C2—C3—C7 | 121.6 (3) | C29—C28—H28 | 119.1 |
| C4—C3—C7 | 119.2 (3) | C27—C28—H28 | 119.1 |
| C5—C4—C3 | 119.8 (3) | C28—C29—C30 | 120.0 (3) |
| C5—C4—H4 | 120.1 | C28—C29—H29 | 120.0 |
| C3—C4—H4 | 120.1 | C30—C29—H29 | 120.0 |
| C6—C5—C4 | 120.7 (3) | C29—C30—C25 | 119.8 (3) |
| C6—C5—H5 | 119.7 | C29—C30—H30 | 120.1 |
| C4—C5—H5 | 119.7 | C25—C30—H30 | 120.1 |
| C5—C6—C1 | 120.4 (3) | C32—C31—C35 | 115.2 (3) |
| C5—C6—H6 | 119.8 | C32—C31—C27 | 121.8 (3) |
| C1—C6—H6 | 119.8 | C35—C31—C27 | 123.0 (3) |
| C8—C7—C11 | 116.9 (3) | C33—C32—C31 | 120.9 (4) |
| C8—C7—C3 | 121.2 (3) | C33—C32—H32 | 119.5 |
| C11—C7—C3 | 121.8 (3) | C31—C32—H32 | 119.5 |
| C9—C8—C7 | 119.7 (4) | N3—C33—C32 | 124.0 (4) |
| C9—C8—H8 | 120.1 | N3—C33—H33 | 118.0 |
| C7—C8—H8 | 120.1 | C32—C33—H33 | 118.0 |
| N1—C9—C8 | 124.1 (4) | N3—C34—C35 | 124.7 (4) |
| N1—C9—H9 | 118.0 | N3—C34—H34 | 117.7 |
| C8—C9—H9 | 118.0 | C35—C34—H34 | 117.7 |
| N1—C10—C11 | 124.5 (4) | C34—C35—C31 | 119.7 (4) |
| N1—C10—H10 | 117.7 | C34—C35—H35 | 120.1 |
| C11—C10—H10 | 117.7 | C31—C35—H35 | 120.1 |
| C10—C11—C7 | 118.8 (4) | O6—C36—O5 | 123.6 (3) |
| C10—C11—H11 | 120.6 | O6—C36—C25 | 118.6 (3) |
| C7—C11—H11 | 120.6 | O5—C36—C25 | 117.8 (3) |
| O1—C12—O2 | 120.2 (3) | | |

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O7—H7*A*···O1$^{i}$ | 0.71 (3) | 2.12 (3) | 2.826 (3) | 173 (4) |
| O7—H7*B*···N1$^{iii}$ | 0.89 (4) | 1.89 (4) | 2.772 (4) | 173 (3) |
| O8—H8*B*···O2$^{ii}$ | 0.75 (3) | 2.05 (3) | 2.793 (3) | 173 (4) |
| O8—H8*A*···N3$^{iv}$ | 0.84 (4) | 1.95 (4) | 2.789 (4) | 175 (3) |

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*; (iii) *x*, *y*−1, *z*−1; (iv) *x*, *y*−1, *z*.