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Poly[[tetraaquatetrakis[μ_3-5-(pyridine-4-carboxamido)isophthalato]cobalt(II)-digadolinium(III)] tetrahydrate]

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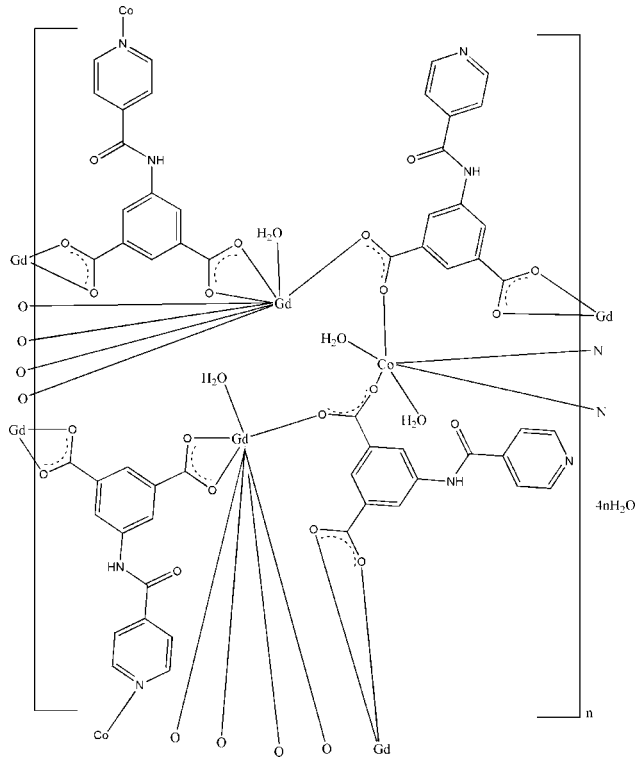
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.031; wR factor = 0.070; data-to-parameter ratio = 11.8.

In the centrosymmetric polymeric title compound, $\{[CoGd_2(C_{14}H_8N_2O_5)_4(H_2O)_4]\cdot 4H_2O\}_n$, the Gd^{III} cation is coordinated by one water molecule and four pyridine-4-carboxamido-isophthalate (L) anions in a distorted square-antiprismatic arrangement, while the Co^{II} cation, located on an inversion center, is coordinated by two pyridyl-N atoms, two carboxylate-O atoms and two water molecules in a distorted octahedral geometry. The asymmetric unit contains two anionic L ligands: one bridges two Gd cations and one Co cation through two carboxyl groups and one pyridine-N atom; the other bridges two Gd cations and one Co cation through two carboxyl groups and the uncoordinated pyridine-N atom is hydrogen-bonded to the adjacent coordinated water molecule. Extensive O—H···O and N—H···O hydrogen bonds are present in the crystal structure.

Related literature

For related hetero-metallic complexes, see: Chen *et al.* (2011); Gu & Xue (2006); Liang *et al.* (2000); Prasad *et al.* (2007); Zhao *et al.* (2003, 2004).



Experimental

Crystal data

$[CoGd_2(C_{14}H_8N_2O_5)_4(H_2O)_4]\cdot 4H_2O$
M_r = 1654.45
Triclinic, $P\overline{1}$
a = 10.1457 (14) Å
b = 10.8728 (15) Å
c = 13.7552 (19) Å
α = 79.123 (2)°
β = 78.844 (3)°
γ = 86.317 (2)°
V = 1461.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.62 mm^{-1}
T = 293 K
0.20 × 0.16 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.622, T_{max} = 0.779
7307 measured reflections
5053 independent reflections
4462 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.070
S = 1.00
5053 reflections
430 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.083 (3)	Gd1—O4^{ii}	2.420 (3)
Co1—O1W	2.178 (4)	Gd1—O6	2.487 (3)
Co1—N4^{i}	2.159 (4)	Gd1—O7	2.408 (3)
Gd1—O2	2.246 (3)	Gd1—O8^{iii}	2.475 (3)
Gd1—O2W	2.365 (3)	Gd1—O9^{iii}	2.382 (3)
Gd1—O3^{ii}	2.436 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4W^{iv}	0.86	2.16	2.999 (6)	166
N3—H3···O4^{v}	0.86	2.15	2.942 (6)	152
O1W—H1WA···O6^{vi}	0.82	2.25	2.992 (5)	151
O1W—H1WB···O3W^{vii}	0.85	2.03	2.753 (6)	143
O2W—H2WA···O3W^{viii}	0.85	2.40	3.130 (6)	144
O2W—H2WB···N2^{i}	0.85	1.92	2.676 (6)	147
O3W—H3WA···O3^{vii}	0.85	1.91	2.737 (6)	163
O3W—H3WB···O8^{iii}	0.85	1.97	2.781 (6)	160
O4W—H4WA···O9^{ix}	0.85	2.26	3.097 (6)	170
O4W—H4WB···O9^{v}	0.85	2.18	3.028 (6)	172

Symmetry codes: (i) $x, y, z-1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+2$; (v) $-x+2, -y+1, -z+2$; (vi) $-x+2, -y+1, -z+1$; (vii) $-x+1, -y+1, -z+1$; (viii) $-x+1, -y, -z+1$; (ix) $x-1, y+1, z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5327).

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supporting information

Acta Cryst. (2011). E**67**, m1431–m1432 [https://doi.org/10.1107/S1600536811038074]

Poly[[tetraaquatetrakis[μ_3-5-(pyridine-4-carboxamido)-isophthalato]cobalt(II)digadolinium(III)] tetrahydrate]

Yi-Fang Deng, Man-Sheng Chen, Chun-Hua Zhang and Dai-Zhi Kuang

S1. Comment

The rational synthesis and investigation of 3d-4f or 4d-4f hetero-metallic complexes are challenge for chemists and have attracted increasing attention in last few years since the competitive reaction containing 3d-4f metal ions in conjunction with ligands often result in formation of a mixture of homometallic assemblies rather than hetero-metallic analogous (Liang *et al.*, 2000; Zhao *et al.*, 2003; Zhao *et al.*, 2004; Gu *et al.*, 2006; Prasad *et al.*, 2007). So we have recently prepared a new lanthanide(III)-transition metal(II) coordination polymer, $[GdCo_{0.5}(H_2O)_2(L)_2]_n.2nH_2O$, (I) through hydro-thermal condition.

In the title compound, the central Gd^{III} ion is eight-coordinated by seven O atoms from four ligands and one water molecule, which forming a distorted square antiprismatic geometry(Fig. 1). It is interesting that the carboxyl groups of two unique L^{2-} ligands exhibit the different coordination modes: one coordinated to two Gd^{III} and one Co^{II} atoms using its two carboxylate groups with μ_1-η^1:η^1-chelate and μ_2-η^1:η^1-bis-monodentate coordination modes while the pyridyl group is free of coordination, the other one coordinated to two Gd^{III} through the carboxylate groups with μ_1-η^1:η^1-chelate coordination mode and one Co^{II} *via* the pyridyl group. Based on the coordination modes of the carboxylate and pyridyl groups of L^{2-} ligands, a complicated three-dimensional network is formed (Fig. 2), which is similar to the complex $\{[LnCo_{0.5}(INAIP)_2(H_2O)_2].2H_2O\}_n$ (Chen, *et al.* 2011).

S2. Experimental

A mixture of 0.05 mmol $Gd(NO_3)_3.6H_2O$ (21.8 mg. 0.05 mmol), H_2L (28.6 mg, 0.1 mmol), $Co(OAc)_2.4H_2O$ (13.1 mg, 0.05 mmol), NaOH (6.0 mg, 0.15 mmol), MeOH (4 ml) and H_2O (6 ml) was heated in a 16 mL capacity Teflon-lined reaction vessel at 433 K for 4 days, the reaction mixture was cooled to room temperature over a period of 40 h. The product was collected by filtration, washed with H_2O and air-dried.

S3. Refinement

H atoms bonded to C atoms were placed geometrically and refined as riding atoms. The pyridyl N atoms were found from a difference Fourier maps and refined as riding, with N—H = 0.86 Å, and the water H atoms were found from Fourier difference maps and refined with restraints for O—H distances (0.82–0.8515 Å) with $U_{iso}(H) = 1.2U_{eq}(O)$.

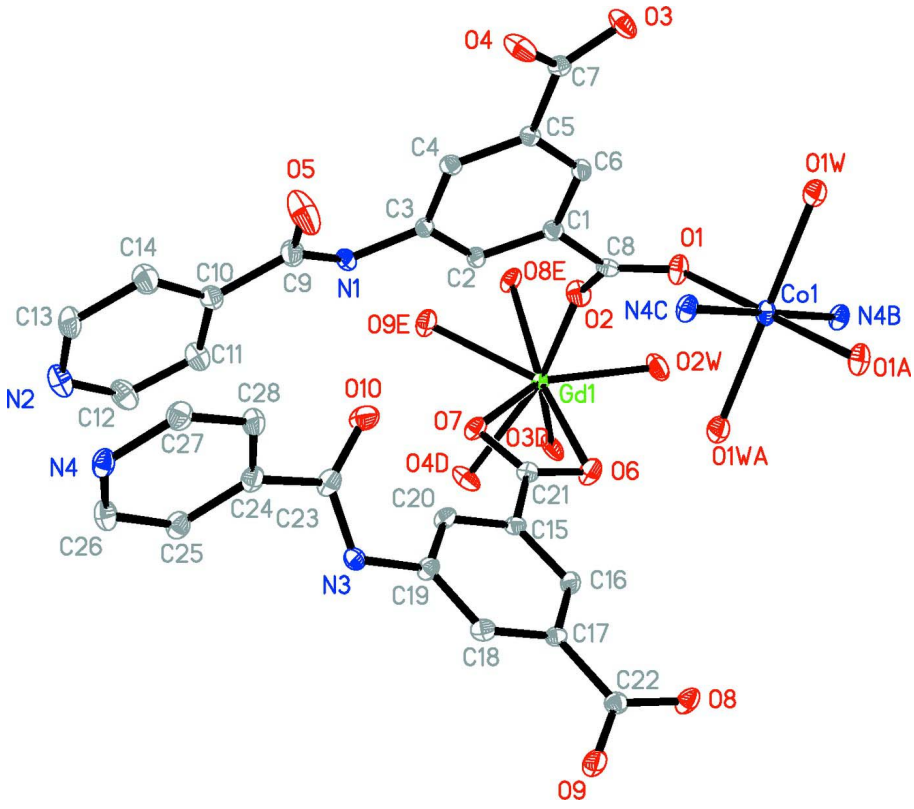

Figure 1

The *ORTEP* drawing of the title compound (I). Displacement ellipsoids are drawn at 30% probability level. [Symmetry codes: (i) 2 - *x*, 1 - *y*, 1 - *z* (ii) 2 - *x*, 1 - *y*, 2 - *z* (iii) *x*, *y*, -1 + *z* (iv) *x*,-1 + *y*, *z* (v)-1 + *x*, *y*, *z*.]

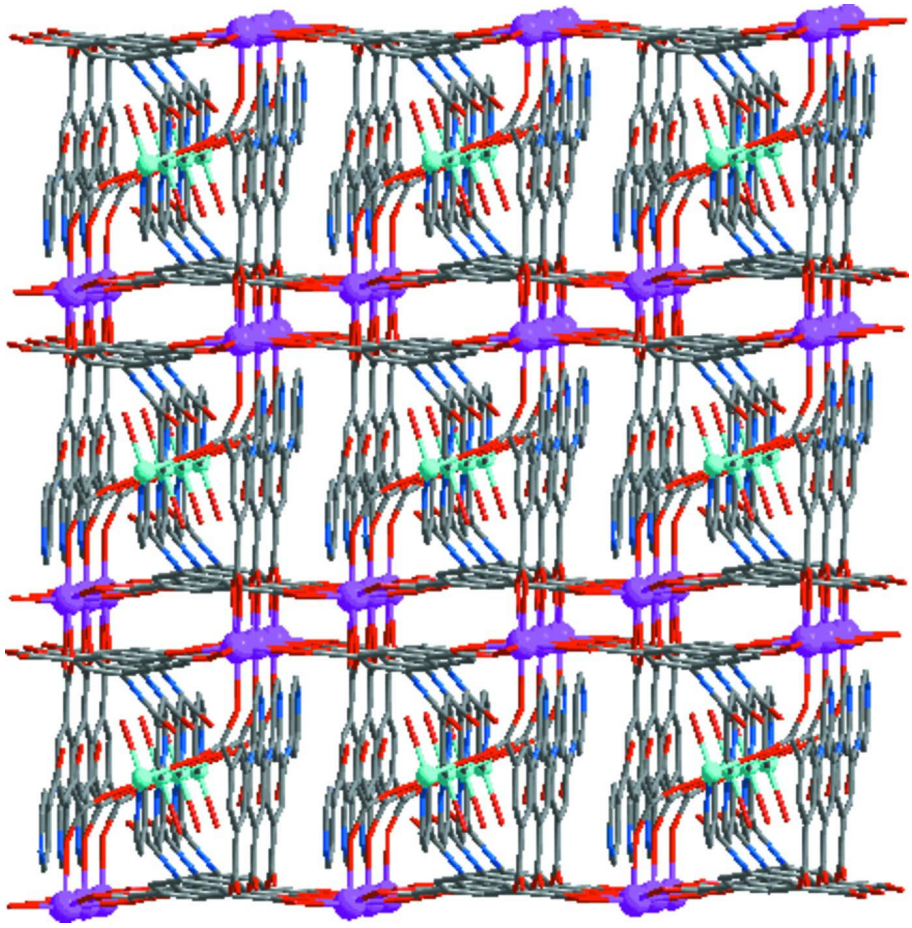

Figure 2

Projection showing the three-dimensional structure of the compound.

Poly[[tetraaquatetrakis[μ_3-5-(pyridine-4- carboxamido)isophthalato]cobalt(II)digadolinium(III)] tetrahydrate]

Crystal data

$[CoGd_2(C_{14}H_8N_2O_5)_4(H_2O)_4]\cdot 4H_2O$
$M_r = 1654.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.1457\ (14)$ Å
$b = 10.8728\ (15)$ Å
$c = 13.7552\ (19)$ Å
$\alpha = 79.123\ (2)°$
$\beta = 78.844\ (3)°$
$\gamma = 86.317\ (2)°$
$V = 1461.3\ (3)$ Å^3
$Z = 1$
$F(000) = 819$
$D_x = 1.880$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5652 reflections
$\theta = 2.7–28.2°$
$\mu = 2.62$ mm^{-1}
$T = 293$ K
Block, pink
0.20 × 0.16 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.622$, $T_{max} = 0.779$
7307 measured reflections
5053 independent reflections

4462 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -12 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.070$
$S = 1.00$
5053 reflections
430 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.88$ 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}
Co1	1.0000	0.5000	0.5000	0.0225 (2)
Gd1	0.68073 (2)	0.07754 (2)	0.702891 (17)	0.01596 (9)
C1	0.7021 (5)	0.4733 (4)	0.7262 (4)	0.0203 (11)
C2	0.6789 (5)	0.4174 (5)	0.8277 (3)	0.0204 (11)
H2	0.6736	0.3308	0.8458	0.024*
C3	0.6639 (4)	0.4907 (4)	0.9019 (3)	0.0193 (11)
C4	0.6653 (4)	0.6204 (4)	0.8743 (4)	0.0197 (11)
H4	0.6539	0.6703	0.9235	0.024*
C5	0.6838 (5)	0.6749 (4)	0.7734 (3)	0.0173 (11)
C6	0.7035 (5)	0.6027 (4)	0.6993 (4)	0.0209 (11)
H6	0.7176	0.6405	0.6317	0.025*
C7	0.6865 (5)	0.8143 (4)	0.7469 (4)	0.0193 (11)
C8	0.7333 (5)	0.3940 (5)	0.6454 (4)	0.0221 (11)
C9	0.6653 (5)	0.4830 (5)	1.0810 (4)	0.0290 (13)
C10	0.6520 (5)	0.4000 (5)	1.1831 (4)	0.0254 (12)
C11	0.6510 (5)	0.2702 (5)	1.2015 (4)	0.0302 (13)
H11	0.6536	0.2269	1.1489	0.036*
C12	0.6462 (5)	0.2065 (5)	1.2977 (4)	0.0354 (14)
H12	0.6463	0.1195	1.3083	0.042*
C13	0.6398 (6)	0.3854 (6)	1.3606 (4)	0.0395 (15)
H13	0.6347	0.4256	1.4152	0.047*
C14	0.6451 (6)	0.4584 (6)	1.2657 (4)	0.0356 (14)

H14	0.6442	0.5454	1.2574	0.043*
C15	1.0257 (5)	0.1207 (4)	0.8319 (4)	0.0196 (11)
C16	1.1577 (5)	0.1051 (4)	0.7839 (4)	0.0224 (11)
H16	1.1755	0.0884	0.7186	0.027*
C17	1.2619 (5)	0.1141 (5)	0.8325 (4)	0.0205 (11)
C18	1.2342 (5)	0.1428 (4)	0.9300 (4)	0.0219 (11)
H18	1.3043	0.1485	0.9634	0.026*
C19	1.1033 (5)	0.1625 (5)	0.9764 (4)	0.0222 (11)
C20	0.9992 (5)	0.1483 (5)	0.9280 (4)	0.0218 (11)
H20	0.9107	0.1574	0.9603	0.026*
C21	0.9089 (5)	0.1090 (4)	0.7833 (4)	0.0209 (11)
C22	1.4062 (5)	0.0983 (5)	0.7846 (4)	0.0230 (12)
C23	0.9939 (5)	0.2964 (5)	1.0919 (4)	0.0265 (12)
C24	0.9909 (5)	0.3393 (5)	1.1902 (4)	0.0257 (12)
C25	0.9824 (5)	0.2572 (5)	1.2814 (4)	0.0269 (12)
H25	0.9817	0.1711	1.2846	0.032*
C26	0.9752 (5)	0.3078 (5)	1.3671 (4)	0.0277 (13)
H26	0.9670	0.2532	1.4286	0.033*
C27	0.9848 (5)	0.5065 (5)	1.2779 (4)	0.0281 (13)
H27	0.9861	0.5923	1.2761	0.034*
C28	0.9885 (5)	0.4655 (5)	1.1898 (4)	0.0271 (12)
H28	0.9895	0.5225	1.1301	0.033*
N1	0.6472 (4)	0.4306 (4)	1.0036 (3)	0.0218 (10)
H1	0.6233	0.3539	1.0173	0.026*
N2	0.6415 (5)	0.2612 (5)	1.3771 (3)	0.0371 (12)
N3	1.0794 (4)	0.2000 (4)	1.0720 (3)	0.0239 (10)
H3	1.1204	0.1604	1.1183	0.029*
N4	0.9793 (4)	0.4299 (4)	1.3671 (3)	0.0246 (10)
O1	0.8077 (3)	0.4368 (3)	0.5644 (2)	0.0302 (9)
O2	0.6813 (4)	0.2877 (3)	0.6641 (3)	0.0322 (9)
O3	0.6714 (4)	0.8704 (3)	0.6616 (3)	0.0351 (10)
O4	0.7066 (4)	0.8773 (3)	0.8103 (3)	0.0358 (10)
O5	0.6911 (5)	0.5913 (4)	1.0738 (3)	0.0564 (13)
O6	0.9267 (3)	0.0946 (3)	0.6916 (3)	0.0312 (9)
O7	0.7925 (3)	0.1148 (3)	0.8335 (2)	0.0242 (8)
O8	1.4396 (3)	0.0994 (4)	0.6915 (3)	0.0301 (9)
O9	1.4954 (3)	0.0854 (4)	0.8378 (3)	0.0413 (11)
O10	0.9241 (4)	0.3512 (4)	1.0332 (3)	0.0392 (10)
O1W	0.9258 (4)	0.6827 (3)	0.4333 (3)	0.0329 (9)
H1WB	0.8653	0.7196	0.4704	0.039*
H1WA	0.9888	0.7243	0.3993	0.039*
O2W	0.7218 (4)	0.0952 (3)	0.5257 (3)	0.0404 (10)
H2WA	0.6782	0.0365	0.5148	0.048*
H2WB	0.6868	0.1627	0.4982	0.048*
O3W	0.3006 (4)	0.1662 (5)	0.5329 (3)	0.0747 (16)
H3WA	0.3248	0.1472	0.4746	0.090*
H3WB	0.3576	0.1389	0.5703	0.090*
O4W	0.4138 (5)	0.8385 (4)	0.9854 (3)	0.0680 (15)

H4WA	0.4328	0.9019	0.9390	0.082*
H4WB	0.4384	0.8526	1.0379	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0265 (6)	0.0248 (6)	0.0171 (5)	−0.0039 (4)	−0.0018 (4)	−0.0071 (4)
Gd1	0.01600 (14)	0.01569 (14)	0.01703 (14)	−0.00071 (9)	−0.00433 (10)	−0.00367 (9)
C1	0.021 (3)	0.020 (3)	0.020 (3)	−0.001 (2)	−0.004 (2)	−0.002 (2)
C2	0.021 (3)	0.017 (3)	0.020 (3)	−0.002 (2)	0.001 (2)	0.000 (2)
C3	0.013 (3)	0.025 (3)	0.018 (3)	0.001 (2)	−0.001 (2)	0.001 (2)
C4	0.016 (3)	0.022 (3)	0.022 (3)	0.001 (2)	−0.006 (2)	−0.004 (2)
C5	0.015 (3)	0.015 (3)	0.020 (3)	−0.003 (2)	−0.003 (2)	−0.001 (2)
C6	0.020 (3)	0.021 (3)	0.019 (3)	−0.002 (2)	−0.002 (2)	−0.001 (2)
C7	0.017 (3)	0.019 (3)	0.023 (3)	0.001 (2)	−0.006 (2)	−0.006 (2)
C8	0.021 (3)	0.020 (3)	0.025 (3)	0.003 (2)	−0.009 (2)	−0.002 (2)
C9	0.028 (3)	0.033 (3)	0.025 (3)	−0.002 (3)	−0.002 (2)	−0.002 (2)
C10	0.018 (3)	0.033 (3)	0.024 (3)	−0.002 (2)	−0.005 (2)	−0.001 (2)
C11	0.036 (3)	0.030 (3)	0.026 (3)	−0.006 (3)	−0.009 (3)	−0.001 (2)
C12	0.039 (4)	0.032 (3)	0.034 (3)	−0.011 (3)	−0.011 (3)	0.004 (3)
C13	0.047 (4)	0.054 (4)	0.020 (3)	0.004 (3)	−0.009 (3)	−0.012 (3)
C14	0.040 (4)	0.037 (4)	0.030 (3)	−0.002 (3)	−0.009 (3)	−0.004 (3)
C15	0.017 (3)	0.021 (3)	0.022 (3)	0.002 (2)	−0.006 (2)	−0.005 (2)
C16	0.024 (3)	0.026 (3)	0.017 (3)	0.001 (2)	−0.004 (2)	−0.006 (2)
C17	0.014 (3)	0.027 (3)	0.021 (3)	0.000 (2)	−0.005 (2)	−0.003 (2)
C18	0.018 (3)	0.025 (3)	0.026 (3)	−0.002 (2)	−0.010 (2)	−0.008 (2)
C19	0.021 (3)	0.026 (3)	0.022 (3)	−0.001 (2)	−0.003 (2)	−0.011 (2)
C20	0.017 (3)	0.026 (3)	0.024 (3)	0.001 (2)	−0.003 (2)	−0.010 (2)
C21	0.023 (3)	0.018 (3)	0.024 (3)	−0.001 (2)	−0.007 (2)	−0.007 (2)
C22	0.024 (3)	0.020 (3)	0.026 (3)	0.000 (2)	−0.005 (2)	−0.004 (2)
C23	0.021 (3)	0.035 (3)	0.026 (3)	−0.004 (2)	−0.003 (2)	−0.013 (3)
C24	0.016 (3)	0.042 (4)	0.022 (3)	0.000 (2)	−0.004 (2)	−0.011 (2)
C25	0.026 (3)	0.034 (3)	0.024 (3)	−0.001 (2)	−0.006 (2)	−0.012 (2)
C26	0.029 (3)	0.032 (3)	0.021 (3)	−0.009 (2)	−0.003 (2)	−0.002 (2)
C27	0.029 (3)	0.027 (3)	0.028 (3)	−0.003 (2)	−0.002 (3)	−0.007 (2)
C28	0.031 (3)	0.033 (3)	0.018 (3)	0.001 (2)	−0.005 (2)	−0.006 (2)
N1	0.025 (2)	0.018 (2)	0.019 (2)	−0.0009 (18)	−0.0032 (19)	0.0015 (18)
N2	0.043 (3)	0.042 (3)	0.026 (3)	−0.009 (2)	−0.010 (2)	0.003 (2)
N3	0.022 (2)	0.033 (3)	0.017 (2)	0.0036 (19)	−0.0085 (19)	−0.0049 (19)
N4	0.021 (2)	0.035 (3)	0.020 (2)	−0.004 (2)	−0.0025 (19)	−0.010 (2)
O1	0.030 (2)	0.039 (2)	0.021 (2)	−0.0097 (18)	0.0009 (17)	−0.0097 (17)
O2	0.048 (2)	0.016 (2)	0.033 (2)	−0.0053 (17)	−0.0041 (19)	−0.0062 (16)
O3	0.070 (3)	0.016 (2)	0.022 (2)	−0.0008 (18)	−0.015 (2)	−0.0015 (15)
O4	0.068 (3)	0.018 (2)	0.030 (2)	0.0048 (18)	−0.028 (2)	−0.0074 (16)
O5	0.113 (4)	0.028 (3)	0.034 (2)	−0.024 (3)	−0.023 (3)	−0.0009 (19)
O6	0.021 (2)	0.052 (3)	0.026 (2)	−0.0032 (17)	−0.0058 (17)	−0.0170 (18)
O7	0.0140 (19)	0.036 (2)	0.026 (2)	−0.0013 (15)	−0.0043 (16)	−0.0138 (16)
O8	0.0164 (19)	0.054 (3)	0.024 (2)	0.0013 (17)	−0.0044 (16)	−0.0168 (18)

O9	0.015 (2)	0.087 (3)	0.022 (2)	0.005 (2)	−0.0068 (17)	−0.010 (2)
O10	0.039 (2)	0.054 (3)	0.032 (2)	0.021 (2)	−0.016 (2)	−0.023 (2)
O1W	0.036 (2)	0.034 (2)	0.026 (2)	0.0018 (17)	0.0009 (17)	−0.0072 (17)
O2W	0.066 (3)	0.031 (2)	0.024 (2)	−0.005 (2)	−0.013 (2)	0.0016 (17)
O3W	0.060 (3)	0.132 (5)	0.031 (3)	0.028 (3)	−0.015 (2)	−0.014 (3)
O4W	0.139 (5)	0.037 (3)	0.030 (2)	−0.031 (3)	−0.015 (3)	−0.003 (2)

Geometric parameters (Å, º)

Co1—O1^{i}	2.083 (3)	C15—C16	1.389 (6)
Co1—O1	2.083 (3)	C15—C21	1.492 (6)
Co1—O1W	2.178 (4)	C16—C17	1.374 (6)
Co1—O1W^{i}	2.178 (4)	C16—H16	0.9300
Co1—N4^{ii}	2.159 (4)	C17—C18	1.406 (6)
Co1—N4^{iii}	2.159 (4)	C17—C22	1.498 (7)
Gd1—O2	2.246 (3)	C18—C19	1.380 (6)
Gd1—O2W	2.365 (3)	C18—H18	0.9300
Gd1—O3^{iv}	2.436 (3)	C19—C20	1.384 (7)
Gd1—O4^{iv}	2.420 (3)	C19—N3	1.421 (6)
Gd1—O6	2.487 (3)	C20—H20	0.9300
Gd1—O7	2.408 (3)	C21—O7	1.252 (5)
Gd1—O8^{v}	2.475 (3)	C21—O6	1.277 (5)
Gd1—O9^{v}	2.382 (3)	C22—O9	1.256 (6)
C1—C6	1.386 (6)	C22—O8	1.257 (6)
C1—C2	1.395 (6)	C23—O10	1.223 (6)
C1—C8	1.505 (7)	C23—N3	1.352 (6)
C2—C3	1.389 (7)	C23—C24	1.506 (7)
C2—H2	0.9300	C24—C28	1.369 (7)
C3—C4	1.390 (6)	C24—C25	1.387 (7)
C3—N1	1.410 (6)	C25—C26	1.380 (7)
C4—C5	1.385 (6)	C25—H25	0.9300
C4—H4	0.9300	C26—N4	1.331 (6)
C5—C6	1.378 (7)	C26—H26	0.9300
C5—C7	1.491 (6)	C27—N4	1.340 (6)
C6—H6	0.9300	C27—C28	1.361 (7)
C7—O3	1.250 (6)	C27—H27	0.9300
C7—O4	1.257 (5)	C28—H28	0.9300
C8—O1	1.246 (5)	N1—H1	0.8600
C8—O2	1.263 (6)	N3—H3	0.8600
C9—O5	1.204 (6)	N4—Co1^{vi}	2.159 (4)
C9—N1	1.345 (6)	O3—Gd1^{vii}	2.436 (3)
C9—C10	1.507 (7)	O4—Gd1^{vii}	2.420 (3)
C10—C11	1.387 (7)	O8—Gd1^{viii}	2.475 (3)
C10—C14	1.390 (7)	O9—Gd1^{viii}	2.382 (3)
C11—C12	1.365 (7)	O1W—H1WB	0.8501
C11—H11	0.9300	O1W—H1WA	0.8200
C12—N2	1.331 (7)	O2W—H2WA	0.8500
C12—H12	0.9300	O2W—H2WB	0.8499

C13—N2	1.326 (7)	O3W—H3WA	0.8515
C13—C14	1.387 (7)	O3W—H3WB	0.8500
C13—H13	0.9300	O4W—H4WA	0.8501
C14—H14	0.9300	O4W—H4WB	0.8501
C15—C20	1.382 (6)		

O1^{i}—Co1—O1	180.00 (19)	O5—C9—C10	118.3 (5)
O1^{i}—Co1—N4^{ii}	87.68 (14)	N1—C9—C10	117.4 (5)
O1—Co1—N4^{ii}	92.32 (14)	C11—C10—C14	117.2 (5)
O1^{i}—Co1—N4^{iii}	92.32 (14)	C11—C10—C9	125.6 (5)
O1—Co1—N4^{iii}	87.68 (14)	C14—C10—C9	117.2 (5)
N4^{ii}—Co1—N4^{iii}	180.000 (1)	C12—C11—C10	119.3 (5)
O1^{i}—Co1—O1W	86.75 (14)	C12—C11—H11	120.3
O1—Co1—O1W	93.25 (14)	C10—C11—H11	120.3
N4^{ii}—Co1—O1W	90.98 (15)	N2—C12—C11	124.1 (5)
N4^{iii}—Co1—O1W	89.02 (15)	N2—C12—H12	117.9
O1^{i}—Co1—O1W^{i}	93.25 (14)	C11—C12—H12	117.9
O1—Co1—O1W^{i}	86.75 (14)	N2—C13—C14	123.2 (5)
N4^{ii}—Co1—O1W^{i}	89.02 (15)	N2—C13—H13	118.4
N4^{iii}—Co1—O1W^{i}	90.98 (15)	C14—C13—H13	118.4
O1W—Co1—O1W^{i}	180.000 (1)	C13—C14—C10	119.2 (6)
O2—Gd1—O2W	82.58 (12)	C13—C14—H14	120.4
O2—Gd1—O9^{v}	91.01 (14)	C10—C14—H14	120.4
O2W—Gd1—O9^{v}	138.94 (13)	C20—C15—C16	119.9 (4)
O2—Gd1—O7	81.95 (12)	C20—C15—C21	117.8 (4)
O2W—Gd1—O7	139.26 (12)	C16—C15—C21	122.2 (4)
O9^{v}—Gd1—O7	78.76 (11)	C17—C16—C15	120.2 (4)
O2—Gd1—O4^{iv}	154.21 (12)	C17—C16—H16	119.9
O2W—Gd1—O4^{iv}	120.60 (12)	C15—C16—H16	119.9
O9^{v}—Gd1—O4^{iv}	78.54 (13)	C16—C17—C18	119.5 (4)
O7—Gd1—O4^{iv}	72.97 (12)	C16—C17—C22	122.6 (4)
O2—Gd1—O3^{iv}	152.78 (12)	C18—C17—C22	117.9 (4)
O2W—Gd1—O3^{iv}	71.09 (12)	C19—C18—C17	120.3 (4)
O9^{v}—Gd1—O3^{iv}	104.19 (13)	C19—C18—H18	119.9
O7—Gd1—O3^{iv}	122.72 (12)	C17—C18—H18	119.9
O4^{iv}—Gd1—O3^{iv}	52.79 (11)	C18—C19—C20	119.4 (4)
O2—Gd1—O8^{v}	85.71 (13)	C18—C19—N3	118.8 (4)
O2W—Gd1—O8^{v}	85.98 (12)	C20—C19—N3	121.8 (4)
O9^{v}—Gd1—O8^{v}	53.03 (11)	C15—C20—C19	120.6 (4)
O7—Gd1—O8^{v}	129.89 (11)	C15—C20—H20	119.7
O4^{iv}—Gd1—O8^{v}	105.71 (13)	C19—C20—H20	119.7
O3^{iv}—Gd1—O8^{v}	85.72 (13)	O7—C21—O6	120.2 (4)
O2—Gd1—O6	84.41 (13)	O7—C21—C15	119.0 (4)
O2W—Gd1—O6	87.95 (12)	O6—C21—C15	120.8 (4)
O9^{v}—Gd1—O6	131.92 (11)	O9—C22—O8	119.4 (5)
O7—Gd1—O6	53.19 (11)	O9—C22—C17	119.6 (4)
O4^{iv}—Gd1—O6	85.28 (13)	O8—C22—C17	121.0 (5)
O3^{iv}—Gd1—O6	100.97 (13)	O9—C22—Gd1^{viii}	57.6 (3)

O8^{v}—Gd1—O6	169.00 (12)	O8—C22—Gd1^{viii}	61.8 (3)
O2—Gd1—C22^{v}	87.78 (13)	C17—C22—Gd1^{viii}	176.5 (3)
O2W—Gd1—C22^{v}	112.54 (14)	O10—C23—N3	123.3 (5)
O9^{v}—Gd1—C22^{v}	26.43 (13)	O10—C23—C24	119.8 (5)
O7—Gd1—C22^{v}	104.25 (13)	N3—C23—C24	116.9 (5)
O4^{iv}—Gd1—C22^{v}	92.60 (14)	C28—C24—C25	118.8 (5)
O3^{iv}—Gd1—C22^{v}	95.88 (14)	C28—C24—C23	118.2 (5)
O8^{v}—Gd1—C22^{v}	26.61 (12)	C25—C24—C23	122.9 (5)
O6—Gd1—C22^{v}	156.94 (13)	C24—C25—C26	117.7 (5)
O2—Gd1—C7^{iv}	178.34 (13)	C24—C25—H25	121.2
O2W—Gd1—C7^{iv}	96.19 (13)	C26—C25—H25	121.2
O9^{v}—Gd1—C7^{iv}	90.65 (14)	N4—C26—C25	124.0 (5)
O7—Gd1—C7^{iv}	98.34 (13)	N4—C26—H26	118.0
O4^{iv}—Gd1—C7^{iv}	26.48 (12)	C25—C26—H26	118.0
O3^{iv}—Gd1—C7^{iv}	26.34 (12)	N4—C27—C28	123.6 (5)
O8^{v}—Gd1—C7^{iv}	95.32 (13)	N4—C27—H27	118.2
O6—Gd1—C7^{iv}	94.44 (13)	C28—C27—H27	118.2
C22^{v}—Gd1—C7^{iv}	93.72 (14)	C27—C28—C24	119.2 (5)
C6—C1—C2	119.9 (4)	C27—C28—H28	120.4
C6—C1—C8	119.6 (4)	C24—C28—H28	120.4
C2—C1—C8	120.5 (4)	C9—N1—C3	125.7 (4)
C3—C2—C1	120.2 (5)	C9—N1—H1	117.2
C3—C2—H2	119.9	C3—N1—H1	117.2
C1—C2—H2	119.9	C12—N2—C13	117.0 (5)
C2—C3—C4	119.5 (4)	C23—N3—C19	121.6 (4)
C2—C3—N1	118.7 (4)	C23—N3—H3	119.2
C4—C3—N1	121.8 (4)	C19—N3—H3	119.2
C5—C4—C3	119.7 (4)	C26—N4—C27	116.6 (4)
C5—C4—H4	120.2	C26—N4—Co1^{vi}	121.8 (3)
C3—C4—H4	120.2	C27—N4—Co1^{vi}	121.3 (3)
C6—C5—C4	121.2 (4)	C8—O1—Co1	144.0 (3)
C6—C5—C7	120.8 (4)	C8—O2—Gd1	155.3 (3)
C4—C5—C7	118.0 (4)	C7—O3—Gd1^{vii}	93.8 (3)
C5—C6—C1	119.5 (5)	C7—O4—Gd1^{vii}	94.4 (3)
C5—C6—H6	120.3	C21—O6—Gd1	91.1 (3)
C1—C6—H6	120.3	C21—O7—Gd1	95.4 (3)
O3—C7—O4	118.8 (4)	C22—O8—Gd1^{viii}	91.5 (3)
O3—C7—C5	121.0 (4)	C22—O9—Gd1^{viii}	96.0 (3)
O4—C7—C5	120.1 (4)	Co1—O1W—H1WB	117.3
O3—C7—Gd1^{vii}	59.9 (2)	Co1—O1W—H1WA	109.9
O4—C7—Gd1^{vii}	59.1 (3)	H1WB—O1W—H1WA	117.8
C5—C7—Gd1^{vii}	177.5 (3)	Gd1—O2W—H2WA	105.0
O1—C8—O2	123.9 (5)	Gd1—O2W—H2WB	110.8
O1—C8—C1	118.6 (4)	H2WA—O2W—H2WB	105.6
O2—C8—C1	117.5 (4)	H3WA—O3W—H3WB	111.2
O5—C9—N1	124.3 (5)	H4WA—O4W—H4WB	107.9
C6—C1—C2—C3	−3.2 (7)	O5—C9—N1—C3	4.4 (9)

C8—C1—C2—C3	173.3 (4)	C10—C9—N1—C3	−175.7 (4)
C1—C2—C3—C4	3.2 (7)	C2—C3—N1—C9	162.1 (5)
C1—C2—C3—N1	−176.9 (4)	C4—C3—N1—C9	−18.1 (7)
C2—C3—C4—C5	−1.0 (7)	C11—C12—N2—C13	0.8 (9)
N1—C3—C4—C5	179.2 (4)	C14—C13—N2—C12	−1.2 (9)
C3—C4—C5—C6	−1.3 (7)	O10—C23—N3—C19	5.8 (8)
C3—C4—C5—C7	−179.2 (4)	C24—C23—N3—C19	−171.8 (4)
C4—C5—C6—C1	1.3 (7)	C18—C19—N3—C23	132.4 (5)
C7—C5—C6—C1	179.2 (4)	C20—C19—N3—C23	−45.9 (7)
C2—C1—C6—C5	0.9 (7)	C25—C26—N4—C27	3.1 (7)
C8—C1—C6—C5	−175.7 (4)	C25—C26—N4—Co1^{vi}	−169.8 (4)
C6—C5—C7—O3	18.9 (7)	C28—C27—N4—C26	−1.1 (8)
C4—C5—C7—O3	−163.2 (5)	C28—C27—N4—Co1^{vi}	171.8 (4)
C6—C5—C7—O4	−159.9 (5)	O2—C8—O1—Co1	−118.9 (5)
C4—C5—C7—O4	18.0 (7)	C1—C8—O1—Co1	61.6 (7)
C6—C1—C8—O1	27.7 (7)	N4^{ii}—Co1—O1—C8	−31.5 (6)
C2—C1—C8—O1	−148.9 (5)	N4^{iii}—Co1—O1—C8	148.5 (6)
C6—C1—C8—O2	−151.9 (5)	O1W—Co1—O1—C8	−122.6 (6)
C2—C1—C8—O2	31.5 (7)	O1W^{i}—Co1—O1—C8	57.4 (6)
O5—C9—C10—C11	−165.6 (5)	O1—C8—O2—Gd1	75.0 (10)
N1—C9—C10—C11	14.5 (8)	C1—C8—O2—Gd1	−105.4 (8)
O5—C9—C10—C14	11.8 (8)	O2W—Gd1—O2—C8	−92.6 (8)
N1—C9—C10—C14	−168.1 (5)	O9^{v}—Gd1—O2—C8	128.1 (8)
C14—C10—C11—C12	−1.3 (8)	O7—Gd1—O2—C8	49.6 (8)
C9—C10—C11—C12	176.1 (5)	O4^{iv}—Gd1—O2—C8	62.9 (9)
C10—C11—C12—N2	0.4 (9)	O3^{iv}—Gd1—O2—C8	−107.1 (8)
N2—C13—C14—C10	0.4 (9)	O8^{v}—Gd1—O2—C8	−179.1 (8)
C11—C10—C14—C13	0.9 (8)	O6—Gd1—O2—C8	−4.0 (8)
C9—C10—C14—C13	−176.7 (5)	C22^{v}—Gd1—O2—C8	154.3 (8)
C20—C15—C16—C17	1.5 (7)	O4—C7—O3—Gd1^{vii}	−4.0 (5)
C21—C15—C16—C17	−178.6 (5)	C5—C7—O3—Gd1^{vii}	177.2 (4)
C15—C16—C17—C18	−1.8 (7)	O3—C7—O4—Gd1^{vii}	4.0 (5)
C15—C16—C17—C22	−179.9 (4)	C5—C7—O4—Gd1^{vii}	−177.2 (4)
C16—C17—C18—C19	−0.4 (7)	O7—C21—O6—Gd1	−3.4 (5)
C22—C17—C18—C19	177.8 (4)	C15—C21—O6—Gd1	177.4 (4)
C17—C18—C19—C20	2.8 (7)	O2—Gd1—O6—C21	86.0 (3)
C17—C18—C19—N3	−175.6 (4)	O2W—Gd1—O6—C21	168.7 (3)
C16—C15—C20—C19	1.0 (7)	O9^{v}—Gd1—O6—C21	−0.3 (4)
C21—C15—C20—C19	−178.9 (5)	O7—Gd1—O6—C21	1.9 (3)
C18—C19—C20—C15	−3.2 (8)	O4^{iv}—Gd1—O6—C21	−70.3 (3)
N3—C19—C20—C15	175.2 (4)	O3^{iv}—Gd1—O6—C21	−121.0 (3)
C20—C15—C21—O7	−5.5 (7)	O8^{v}—Gd1—O6—C21	112.2 (6)
C16—C15—C21—O7	174.6 (4)	C22^{v}—Gd1—O6—C21	15.2 (5)
C20—C15—C21—O6	173.8 (4)	C7^{iv}—Gd1—O6—C21	−95.2 (3)
C16—C15—C21—O6	−6.1 (7)	O6—C21—O7—Gd1	3.5 (5)
C16—C17—C22—O9	−167.4 (5)	C15—C21—O7—Gd1	−177.2 (4)
C18—C17—C22—O9	14.5 (7)	O2—Gd1—O7—C21	−91.0 (3)
C16—C17—C22—O8	13.5 (7)	O2W—Gd1—O7—C21	−22.3 (4)

C18—C17—C22—O8	−164.7 (5)	O9^{v}—Gd1—O7—C21	176.4 (3)
O10—C23—C24—C28	−41.3 (7)	O4^{iv}—Gd1—O7—C21	95.1 (3)
N3—C23—C24—C28	136.4 (5)	O3^{iv}—Gd1—O7—C21	76.6 (3)
O10—C23—C24—C25	134.8 (6)	O8^{v}—Gd1—O7—C21	−168.4 (3)
N3—C23—C24—C25	−47.5 (7)	O6—Gd1—O7—C21	−1.9 (3)
C28—C24—C25—C26	−1.5 (7)	C22^{v}—Gd1—O7—C21	−176.6 (3)
C23—C24—C25—C26	−177.5 (5)	C7^{iv}—Gd1—O7—C21	87.4 (3)
C24—C25—C26—N4	−1.8 (8)	O9—C22—O8—Gd1^{viii}	−1.6 (5)
N4—C27—C28—C24	−2.0 (8)	C17—C22—O8—Gd1^{viii}	177.6 (4)
C25—C24—C28—C27	3.3 (8)	O8—C22—O9—Gd1^{viii}	1.6 (5)
C23—C24—C28—C27	179.5 (5)	C17—C22—O9—Gd1^{viii}	−177.5 (4)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) *x*, *y*, *z*−1; (iv) *x*, *y*−1, *z*; (v) *x*−1, *y*, *z*; (vi) *x*, *y*, *z*+1; (vii) *x*, *y*+1, *z*; (viii) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4*W*^{ix}	0.86	2.16	2.999 (6)	166
N3—H3···O4^{ii}	0.86	2.15	2.942 (6)	152
O1*W*—H1*WA*···O6^{i}	0.82	2.25	2.992 (5)	151
O1*W*—H1*WB*···O3*W*^{x}	0.85	2.03	2.753 (6)	143
O2*W*—H2*WA*···O3*W*^{xi}	0.85	2.40	3.130 (6)	144
O2*W*—H2*WB*···N2^{iii}	0.85	1.92	2.676 (6)	147
O3*W*—H3*WA*···O3^{x}	0.85	1.91	2.737 (6)	163
O3*W*—H3*WB*···O8^{v}	0.85	1.97	2.781 (6)	160
O4*W*—H4*WA*···O9^{xii}	0.85	2.26	3.097 (6)	170
O4*W*—H4*WB*···O9^{ii}	0.85	2.18	3.028 (6)	172

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) *x*, *y*, *z*−1; (v) *x*−1, *y*, *z*; (ix) −*x*+1, −*y*+1, −*z*+2; (x) −*x*+1, −*y*+1, −*z*+1; (xi) −*x*+1, −*y*, −*z*+1; (xii) *x*−1, *y*+1, *z*.