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Bis(guanidinium) tris(pyridine-2,6-dicarboxylato-κ^3O^2,N,O^6)zirconate(II) tetrahydrate

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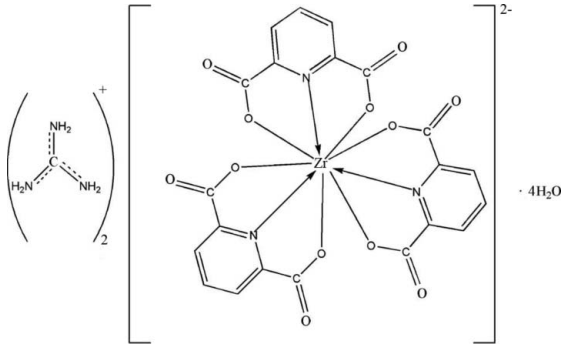
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.146; data-to-parameter ratio = 18.5.

In the title complex, $(CH_6N_3)_2[Zr(C_7H_3NO_4)_3]\cdot 4H_2O$, the Zr^{IV} ion lies on a twofold rotation axes and is coordinated by six O and three N atoms of three tridentate pyridine-2,6-dicarboxylate ligands, forming a slightly distorted tricapped trigonal–prismatic geometry. In the crystal, O—H···O and N—H···O hydrogen bonds link the components into a three-dimensional network.

Related literature

For related structures, see: Aghabozorg *et al.* (2005); Tabatabaee (2010); Tabatabaee *et al.* (2009, 2011*a*,*b*,*c*, 2012); Derikvand *et al.* (2010); Attar Gharamaleki *et al.* (2009).



Experimental

Crystal data

$(CH_6N_3)_2[Zr(C_7H_3NO_4)_3]\cdot 4H_2O$
M_r = 778.77
Orthorhombic, *Pbcn*
a = 17.2444 (9) Å
b = 10.8583 (5) Å
c = 16.5268 (8) Å
V = 3094.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 120 K
0.17 × 0.15 × 0.07 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.884, T_{max} = 0.970
32229 measured reflections
4116 independent reflections
2884 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.146
S = 1.07
4116 reflections
223 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*NA*···O1	0.77	2.23	3.003 (4)	175
N3—H3*NB*···O2W^{i}	0.86	2.15	2.930 (4)	150
N4—H4*NA*···O2W^{i}	0.83	2.04	2.818 (4)	156
N4—H4*NB*···O1W^{ii}	0.78	2.06	2.834 (4)	175
N5—H5*NA*···O2	0.88	1.95	2.828 (4)	171
N5—H5*NB*···O3^{iii}	0.79	2.45	3.143 (4)	148
N5—H5*NB*···O4^{iii}	0.79	2.52	3.171 (4)	141
O1*W*—H1*WA*···O3^{iv}	0.84	2.33	3.041 (3)	143
O1*W*—H1*WA*···O5^{iv}	0.84	2.38	3.076 (3)	140
O1*W*—H1*WB*···O6	0.89	1.87	2.761 (3)	175
O2*W*—H2*WA*···O5^{iv}	0.86	2.07	2.909 (3)	165
O2*W*—H2*WA*···O6^{iv}	0.86	2.57	3.085 (3)	119
O2*W*—H2*WB*···O4^{v}	0.94	1.84	2.745 (3)	160

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*, *DIAMOND* (Brandenburg, 1999) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

The authors wish to express their deepest appreciation to the late Professor Dr. H Aghabozorg who has inspired, advised and assisted during this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5430).

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supporting information

Acta Cryst. (2012). E**68**, m462–m463 [https://doi.org/10.1107/S1600536812011439]

Bis(guanidinium) tris(pyridine-2,6-dicarboxylato-κ^3O^2,N,O^6)zirconate(II) tetrahydrate

Masoumeh Tabatabaee, Mahnaz Adineh, Zohreh Derikvand and Jafar Attar Gharamaleki

S1. Comment

In recent years, our research group has been interested in the synthesis of proton transfer compounds and study of their behavior with metal ions. We have focused on the proton delivery of polycarboxylic acids. Pyridine-2,6-dicarboxylic acid ($pydcH_2$) is a very important carboxylate derivative and has attracted much interest in coordination chemistry. This is the acid we have utilized widely in our studies (Tabatabaee *et al.*, 2010, 2011*a*, 2011*b*, 2011*c*, 2012; Derikvand *et al.*, 2010; Attar Gharamaleki *et al.*, 2009). In this paper we report the crystal structure of the title complex (I). The Zr^{IV} ion lies on a twofold rotation axis. The asymmetric unit and the symmetry complete cation is shown in Fig. 1. The Zr^{IV} atom is coordinated by three tridentate pydc ligands forming a slightly distorted tricapped trigonal prismatic environment (Fig. 2). The Zr—N distances and Zr—O distances are consistent with those found in $(pydaH)_2[Zr(pydc)_3].5H_2O$ (Aghabozorg *et al.*, 2005). In the crystal, O—H···O and N—H···O hydrogen bonds (Table 1) link the components into a three-dimensional network (Fig. 3).

S2. Experimental

An aqueous solution of $ZrOCl_2.8H_2O$, (161 mg, 0.5 mmol) in water (5 ml) was added to a stirring solution of (20 ml) pyridine-2,6-dicarboxylic acid (176 mg, 1 mmol) and guanidine hydrochloride (95 mg, 1 mmol). The reaction mixture was stirred at 298K for 1 h. Colorless crystals of the title compound were obtained after 4 days by slow evaporation of the solvent at room temperature.

S3. Refinement

H atoms bonded to C atoms were placed in calculated positions. The H atoms of water molecules and NH_2 groups were located in difference Fourier maps and included in 'as found′ positions. All hydrogen atoms were refined in isotropic approximatiom in a riding-model approximation with U_{iso}(H) parameters equal to 1.2 U_{eq}(C), 1.5 U_{eq}(O,*N*).

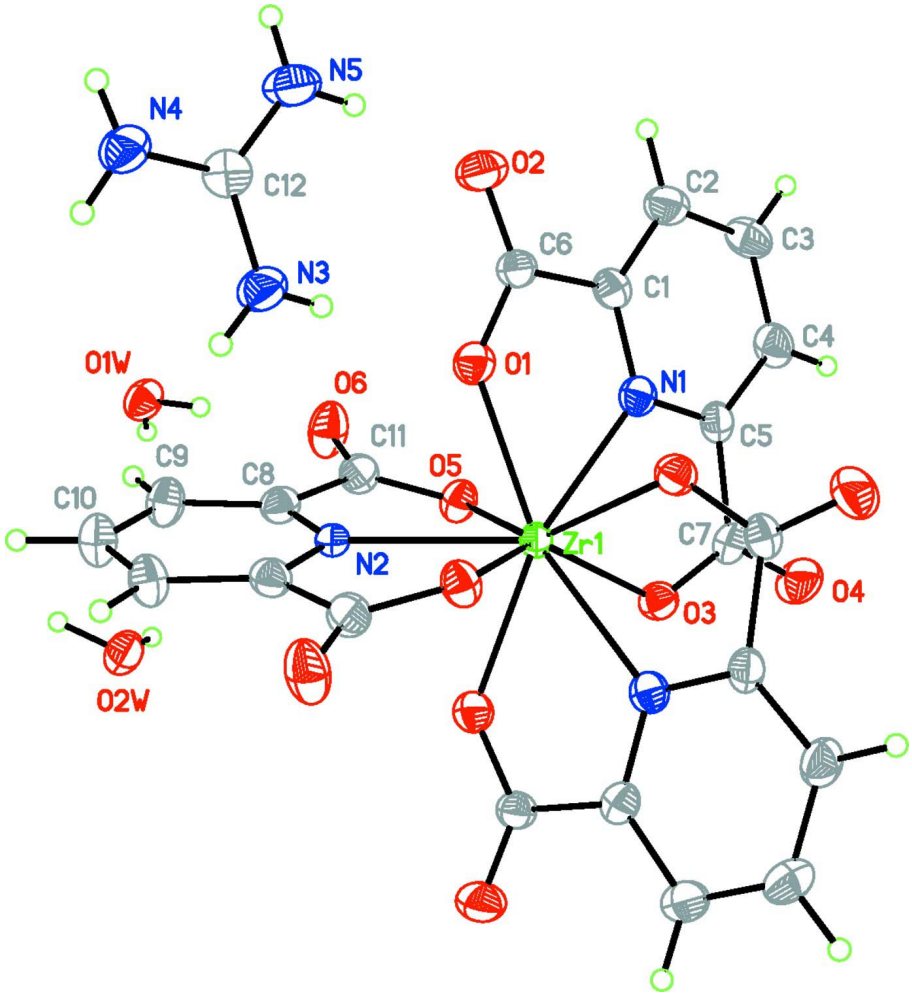

Figure 1

The molecular structure of (I) with ellipsoids drawn at the 50% probability level. The unlabeled atoms are related by the symmetry operator (-x+1, y, -z+1/2). Only the symmetry unique anions and water molecules are shown.

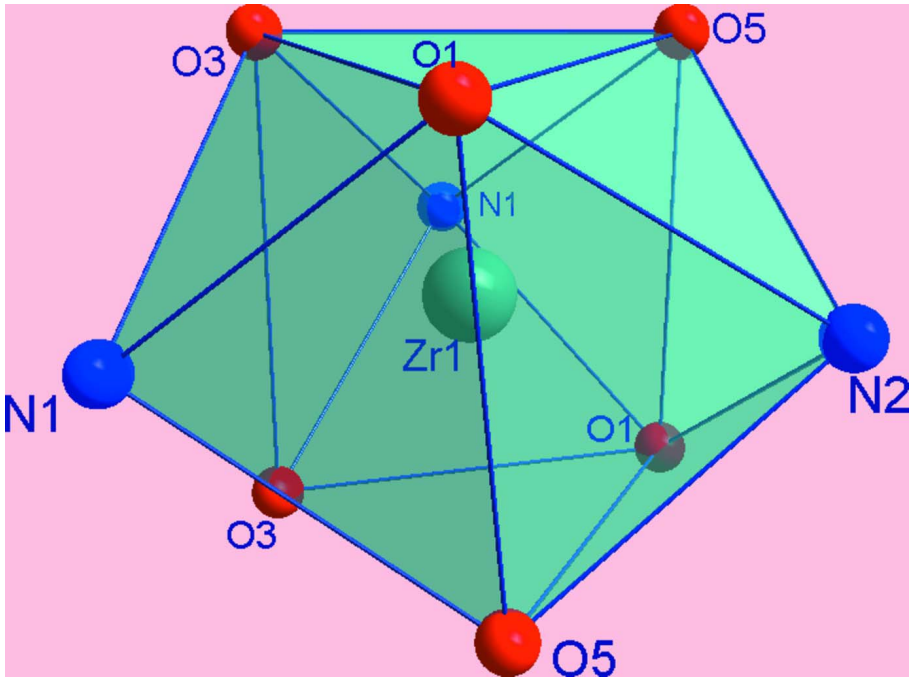

Figure 2

View of the coordination environment of the Zr^{IV} ion.

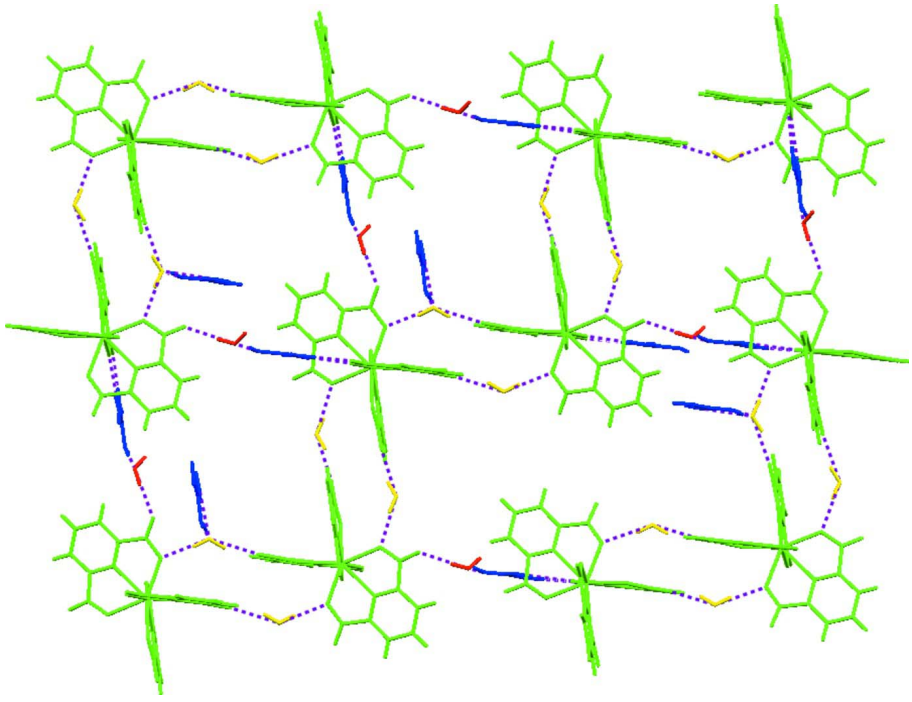

Figure 3

Part of the crystal structure of (I). The donor to acceptor distances of the hydrogen bonds are shown as dotted lines.

Bis(guanidinium) tris(pyridine-2,6-dicarboxylato- κ^3O^2,N,O^6)zirconate(II) tetrahydrate

Crystal data

$(CH_6N_3)_2[Zr(C_7H_3NO_4)_3]\cdot 4H_2O$
$M_r = 778.77$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 17.2444$ (9) Å
$b = 10.8583$ (5) Å
$c = 16.5268$ (8) Å
$V = 3094.6$ (3) Å^3
$Z = 4$
$F(000) = 1592$
$D_x = 1.672$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4151 reflections
$\theta = 2.3$–$26.0°$
$\mu = 0.45$ mm^{-1}
$T = 120$ K
Prism, colorless
0.17 × 0.15 × 0.07 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.884$, $T_{max} = 0.970$
32229 measured reflections
4116 independent reflections
2884 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 29.0°$, $\theta_{min} = 2.2°$
$h = -23\rightarrow23$
$k = -14\rightarrow14$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.146$
$S = 1.07$
4116 reflections
223 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 8.430P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zr1	0.5000	0.72625 (4)	0.2500	0.01631 (13)
O1	0.38154 (13)	0.6592 (2)	0.28200 (14)	0.0245 (5)
O2	0.25204 (15)	0.6675 (3)	0.27362 (17)	0.0349 (6)
O3	0.54360 (12)	0.8668 (2)	0.16530 (13)	0.0226 (5)
O4	0.53142 (16)	1.0370 (2)	0.09047 (17)	0.0362 (6)

O5	0.47334 (14)	0.6443 (2)	0.12914 (14)	0.0236 (5)
O6	0.42065 (17)	0.4926 (2)	0.05627 (15)	0.0354 (6)
N1	0.40034 (15)	0.8418 (2)	0.18731 (16)	0.0214 (5)
N2	0.5000	0.5072 (3)	0.2500	0.0171 (7)
C1	0.32630 (19)	0.8123 (3)	0.20019 (19)	0.0225 (6)
C2	0.2655 (2)	0.8764 (3)	0.1641 (2)	0.0292 (7)
H2A	0.2131	0.8533	0.1731	0.035*
C3	0.2842 (2)	0.9750 (3)	0.1146 (2)	0.0295 (7)
H3A	0.2441	1.0216	0.0898	0.035*
C4	0.3609 (2)	1.0061 (3)	0.1010 (2)	0.0273 (7)
H4A	0.3743	1.0733	0.0670	0.033*
C5	0.41742 (19)	0.9359 (3)	0.13861 (19)	0.0219 (6)
C6	0.31649 (18)	0.7054 (3)	0.25566 (19)	0.0218 (6)
C7	0.50369 (18)	0.9516 (3)	0.12932 (18)	0.0205 (6)
C8	0.47612 (18)	0.4462 (3)	0.18438 (19)	0.0222 (6)
C9	0.4742 (2)	0.3187 (3)	0.1823 (2)	0.0273 (7)
H9A	0.4557	0.2761	0.1360	0.033*
C10	0.5000	0.2551 (4)	0.2500	0.0284 (10)
H10A	0.5000	0.1676	0.2500	0.034*
C11	0.45375 (19)	0.5307 (3)	0.1163 (2)	0.0240 (6)
N3	0.33875 (17)	0.4432 (3)	0.38628 (19)	0.0312 (7)
H3NA	0.3482	0.5016	0.3616	0.047*
H3NB	0.3752	0.4039	0.4112	0.047*
N4	0.25724 (18)	0.3150 (3)	0.45574 (18)	0.0314 (7)
H4NA	0.2971	0.2749	0.4652	0.047*
H4NB	0.2158	0.2885	0.4626	0.047*
N5	0.20814 (17)	0.4727 (3)	0.3776 (2)	0.0364 (8)
H5NA	0.2166	0.5344	0.3439	0.055*
H5NB	0.1654	0.4517	0.3865	0.055*
C12	0.26720 (19)	0.4098 (3)	0.4060 (2)	0.0268 (7)
O1W	0.39648 (14)	0.2667 (2)	−0.01609 (15)	0.0279 (5)
H1WA	0.4195	0.2642	−0.0607	0.042*
H1WB	0.4026	0.3377	0.0100	0.042*
O2W	0.58669 (15)	0.2479 (2)	0.01935 (16)	0.0310 (6)
H2WA	0.5768	0.2747	−0.0287	0.047*
H2WB	0.5631	0.1722	0.0319	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.0173 (2)	0.0148 (2)	0.0169 (2)	0.000	−0.00061 (15)	0.000
O1	0.0241 (12)	0.0232 (11)	0.0261 (11)	−0.0009 (9)	−0.0003 (9)	0.0031 (9)
O2	0.0217 (12)	0.0369 (15)	0.0462 (15)	−0.0031 (11)	0.0017 (11)	0.0095 (12)
O3	0.0213 (11)	0.0233 (11)	0.0232 (11)	−0.0011 (9)	0.0001 (9)	0.0015 (9)
O4	0.0327 (13)	0.0314 (14)	0.0444 (15)	−0.0070 (11)	−0.0008 (12)	0.0144 (12)
O5	0.0280 (11)	0.0211 (11)	0.0216 (11)	−0.0035 (9)	−0.0030 (9)	0.0003 (9)
O6	0.0521 (16)	0.0249 (12)	0.0292 (13)	−0.0054 (11)	−0.0141 (12)	−0.0004 (10)
N1	0.0231 (13)	0.0206 (13)	0.0205 (13)	−0.0005 (10)	0.0002 (10)	−0.0013 (10)

N2	0.0149 (15)	0.0161 (16)	0.0203 (16)	0.000	0.0013 (13)	0.000
C1	0.0236 (15)	0.0212 (14)	0.0228 (15)	0.0026 (12)	−0.0013 (12)	0.0011 (12)
C2	0.0220 (16)	0.0310 (18)	0.0345 (19)	0.0021 (13)	−0.0010 (14)	0.0036 (15)
C3	0.0256 (17)	0.0336 (18)	0.0294 (17)	0.0077 (14)	−0.0024 (14)	0.0045 (15)
C4	0.0311 (17)	0.0233 (16)	0.0276 (16)	0.0032 (13)	−0.0045 (13)	0.0055 (13)
C5	0.0260 (15)	0.0163 (14)	0.0235 (15)	0.0008 (12)	−0.0029 (12)	−0.0002 (12)
C6	0.0192 (14)	0.0226 (15)	0.0235 (15)	−0.0006 (11)	0.0006 (12)	−0.0015 (12)
C7	0.0258 (15)	0.0177 (13)	0.0179 (13)	−0.0029 (12)	−0.0011 (12)	−0.0001 (11)
C8	0.0199 (14)	0.0238 (16)	0.0230 (15)	−0.0014 (12)	0.0018 (11)	−0.0023 (13)
C9	0.0365 (18)	0.0214 (16)	0.0239 (16)	−0.0030 (14)	−0.0006 (13)	−0.0025 (13)
C10	0.040 (3)	0.020 (2)	0.025 (2)	0.000	−0.003 (2)	0.000
C11	0.0244 (15)	0.0240 (16)	0.0235 (15)	−0.0002 (12)	−0.0027 (12)	−0.0022 (12)
N3	0.0240 (14)	0.0321 (16)	0.0375 (17)	−0.0040 (12)	0.0005 (12)	0.0113 (13)
N4	0.0269 (15)	0.0324 (16)	0.0348 (16)	−0.0033 (12)	0.0041 (12)	0.0093 (13)
N5	0.0208 (14)	0.0441 (19)	0.0444 (19)	−0.0014 (13)	0.0018 (13)	0.0160 (15)
C12	0.0275 (17)	0.0300 (17)	0.0228 (16)	−0.0002 (14)	−0.0002 (12)	0.0000 (13)
O1W	0.0299 (12)	0.0258 (12)	0.0280 (12)	−0.0058 (10)	0.0040 (10)	−0.0057 (10)
O2W	0.0336 (13)	0.0273 (12)	0.0323 (13)	−0.0075 (10)	−0.0053 (11)	0.0050 (10)

Geometric parameters (Å, º)

Zr1—O3	2.203 (2)	C3—H3A	0.9500
Zr1—O3^{i}	2.203 (2)	C4—C5	1.384 (4)
Zr1—O1^{i}	2.232 (2)	C4—H4A	0.9500
Zr1—O1	2.232 (2)	C5—C7	1.505 (4)
Zr1—O5	2.234 (2)	C8—C9	1.384 (5)
Zr1—O5^{i}	2.234 (2)	C8—C11	1.503 (5)
Zr1—N1^{i}	2.366 (3)	C9—C10	1.388 (4)
Zr1—N1	2.366 (3)	C9—H9A	0.9500
Zr1—N2	2.378 (4)	C10—C9^{i}	1.388 (4)
O1—C6	1.304 (4)	C10—H10A	0.9500
O2—C6	1.222 (4)	N3—C12	1.327 (4)
O3—C7	1.294 (4)	N3—H3NA	0.7713
O4—C7	1.225 (4)	N3—H3NB	0.8647
O5—C11	1.297 (4)	N4—C12	1.329 (4)
O6—C11	1.217 (4)	N4—H4NA	0.8289
N1—C1	1.333 (4)	N4—H4NB	0.7790
N1—C5	1.334 (4)	N5—C12	1.312 (4)
N2—C8	1.336 (4)	N5—H5NA	0.8832
N2—C8^{i}	1.336 (4)	N5—H5NB	0.7861
C1—C2	1.393 (5)	O1W—H1WA	0.8370
C1—C6	1.489 (5)	O1W—H1WB	0.8899
C2—C3	1.386 (5)	O2W—H2WA	0.8620
C2—H2A	0.9500	O2W—H2WB	0.9408
C3—C4	1.382 (5)		

O3—Zr1—O3^{i}	92.30 (12)	N1—C1—C6	113.2 (3)
O3—Zr1—O1^{i}	76.29 (8)	C2—C1—C6	124.6 (3)

O3^{i}—Zr1—O1^{i}	133.53 (8)	C3—C2—C1	117.6 (3)
O3—Zr1—O1	133.53 (8)	C3—C2—H2A	121.2
O3^{i}—Zr1—O1	76.29 (8)	C1—C2—H2A	121.2
O1^{i}—Zr1—O1	141.94 (12)	C4—C3—C2	120.5 (3)
O3—Zr1—O5	77.18 (8)	C4—C3—H3A	119.8
O3^{i}—Zr1—O5	140.67 (8)	C2—C3—H3A	119.8
O1^{i}—Zr1—O5	81.18 (9)	C3—C4—C5	117.8 (3)
O1—Zr1—O5	83.89 (9)	C3—C4—H4A	121.1
O3—Zr1—O5^{i}	140.67 (8)	C5—C4—H4A	121.1
O3^{i}—Zr1—O5^{i}	77.18 (8)	N1—C5—C4	122.5 (3)
O1^{i}—Zr1—O5^{i}	83.89 (9)	N1—C5—C7	111.5 (3)
O1—Zr1—O5^{i}	81.18 (9)	C4—C5—C7	126.0 (3)
O5—Zr1—O5^{i}	133.07 (12)	O2—C6—O1	124.9 (3)
O3—Zr1—N1^{i}	70.31 (8)	O2—C6—C1	121.0 (3)
O3^{i}—Zr1—N1^{i}	66.58 (8)	O1—C6—C1	114.1 (3)
O1^{i}—Zr1—N1^{i}	67.17 (9)	O4—C7—O3	124.9 (3)
O1—Zr1—N1^{i}	137.20 (9)	O4—C7—C5	121.7 (3)
O5—Zr1—N1^{i}	138.75 (9)	O3—C7—C5	113.4 (3)
O5^{i}—Zr1—N1^{i}	70.75 (9)	N2—C8—C9	121.6 (3)
O3—Zr1—N1	66.58 (8)	N2—C8—C11	112.6 (3)
O3^{i}—Zr1—N1	70.31 (8)	C9—C8—C11	125.9 (3)
O1^{i}—Zr1—N1	137.20 (9)	C8—C9—C10	118.1 (3)
O1—Zr1—N1	67.17 (9)	C8—C9—H9A	121.0
O5—Zr1—N1	70.75 (9)	C10—C9—H9A	121.0
O5^{i}—Zr1—N1	138.75 (9)	C9—C10—C9^{i}	120.2 (4)
N1^{i}—Zr1—N1	115.98 (13)	C9—C10—H10A	119.9
O3—Zr1—N2	133.85 (6)	C9^{i}—C10—H10A	119.9
O3^{i}—Zr1—N2	133.85 (6)	O6—C11—O5	125.4 (3)
O1^{i}—Zr1—N2	70.97 (6)	O6—C11—C8	121.6 (3)
O1—Zr1—N2	70.97 (6)	O5—C11—C8	113.1 (3)
O5—Zr1—N2	66.54 (6)	C12—N3—H3NA	123.4
O5^{i}—Zr1—N2	66.54 (6)	C12—N3—H3NB	115.1
N1^{i}—Zr1—N2	122.01 (6)	H3NA—N3—H3NB	120.4
N1—Zr1—N2	122.01 (6)	C12—N4—H4NA	114.6
C6—O1—Zr1	125.7 (2)	C12—N4—H4NB	119.6
C7—O3—Zr1	127.11 (19)	H4NA—N4—H4NB	122.8
C11—O5—Zr1	125.4 (2)	C12—N5—H5NA	119.5
C1—N1—C5	119.5 (3)	C12—N5—H5NB	120.7
C1—N1—Zr1	119.9 (2)	H5NA—N5—H5NB	119.5
C5—N1—Zr1	120.7 (2)	N5—C12—N3	119.5 (3)
C8—N2—C8^{i}	120.5 (4)	N5—C12—N4	121.6 (3)
C8—N2—Zr1	119.8 (2)	N3—C12—N4	118.9 (3)
C8^{i}—N2—Zr1	119.8 (2)	H1WA—O1W—H1WB	113.4
N1—C1—C2	122.2 (3)	H2WA—O2W—H2WB	114.3

O3—Zr1—O1—C6	−5.4 (3)	O3—Zr1—N2—C8^{i}	130.96 (17)
O3^{i}—Zr1—O1—C6	74.6 (2)	O3^{i}—Zr1—N2—C8^{i}	−49.04 (17)
O1^{i}—Zr1—O1—C6	−138.4 (3)	O1^{i}—Zr1—N2—C8^{i}	83.72 (17)

O5—Zr1—O1—C6	−71.2 (3)	O1—Zr1—N2—C8^{i}	−96.28 (17)
O5^{i}—Zr1—O1—C6	153.4 (3)	O5—Zr1—N2—C8^{i}	172.17 (17)
N1^{i}—Zr1—O1—C6	104.6 (3)	O5^{i}—Zr1—N2—C8^{i}	−7.83 (17)
N1—Zr1—O1—C6	0.5 (2)	N1^{i}—Zr1—N2—C8^{i}	38.12 (17)
N2—Zr1—O1—C6	−138.4 (3)	N1—Zr1—N2—C8^{i}	−141.88 (17)
O3^{i}—Zr1—O3—C7	−59.3 (2)	C5—N1—C1—C2	0.3 (5)
O1^{i}—Zr1—O3—C7	166.3 (3)	Zr1—N1—C1—C2	−179.3 (2)
O1—Zr1—O3—C7	13.9 (3)	C5—N1—C1—C6	179.9 (3)
O5—Zr1—O3—C7	82.4 (2)	Zr1—N1—C1—C6	0.4 (4)
O5^{i}—Zr1—O3—C7	−131.8 (2)	N1—C1—C2—C3	−1.2 (5)
N1^{i}—Zr1—O3—C7	−123.4 (3)	C6—C1—C2—C3	179.2 (3)
N1—Zr1—O3—C7	8.1 (2)	C1—C2—C3—C4	1.1 (5)
N2—Zr1—O3—C7	120.7 (2)	C2—C3—C4—C5	−0.2 (5)
O3—Zr1—O5—C11	166.3 (3)	C1—N1—C5—C4	0.7 (5)
O3^{i}—Zr1—O5—C11	−116.0 (3)	Zr1—N1—C5—C4	−179.7 (2)
O1^{i}—Zr1—O5—C11	88.4 (3)	C1—N1—C5—C7	−177.9 (3)
O1—Zr1—O5—C11	−56.4 (3)	Zr1—N1—C5—C7	1.7 (3)
O5^{i}—Zr1—O5—C11	15.4 (2)	C3—C4—C5—N1	−0.7 (5)
N1^{i}—Zr1—O5—C11	127.9 (2)	C3—C4—C5—C7	177.7 (3)
N1—Zr1—O5—C11	−124.3 (3)	Zr1—O1—C6—O2	179.8 (3)
N2—Zr1—O5—C11	15.4 (2)	Zr1—O1—C6—C1	−0.4 (4)
O3—Zr1—N1—C1	175.0 (3)	N1—C1—C6—O2	179.8 (3)
O3^{i}—Zr1—N1—C1	−83.4 (2)	C2—C1—C6—O2	−0.6 (5)
O1^{i}—Zr1—N1—C1	143.0 (2)	N1—C1—C6—O1	0.0 (4)
O1—Zr1—N1—C1	−0.4 (2)	C2—C1—C6—O1	179.7 (3)
O5—Zr1—N1—C1	91.0 (2)	Zr1—O3—C7—O4	170.7 (2)
O5^{i}—Zr1—N1—C1	−43.3 (3)	Zr1—O3—C7—C5	−9.9 (4)
N1^{i}—Zr1—N1—C1	−133.3 (3)	N1—C5—C7—O4	−176.1 (3)
N2—Zr1—N1—C1	46.7 (3)	C4—C5—C7—O4	5.4 (5)
O3—Zr1—N1—C5	−4.5 (2)	N1—C5—C7—O3	4.5 (4)
O3^{i}—Zr1—N1—C5	97.1 (2)	C4—C5—C7—O3	−174.0 (3)
O1^{i}—Zr1—N1—C5	−36.6 (3)	C8^{i}—N2—C8—C9	0.9 (2)
O1—Zr1—N1—C5	−180.0 (3)	Zr1—N2—C8—C9	−179.1 (2)
O5—Zr1—N1—C5	−88.5 (2)	C8^{i}—N2—C8—C11	−178.4 (3)
O5^{i}—Zr1—N1—C5	137.1 (2)	Zr1—N2—C8—C11	1.6 (3)
N1^{i}—Zr1—N1—C5	47.2 (2)	N2—C8—C9—C10	−1.8 (5)
N2—Zr1—N1—C5	−132.8 (2)	C11—C8—C9—C10	177.4 (3)
O3—Zr1—N2—C8	−49.04 (17)	C8—C9—C10—C9^{i}	0.9 (2)
O3^{i}—Zr1—N2—C8	130.96 (17)	Zr1—O5—C11—O6	160.2 (3)
O1^{i}—Zr1—N2—C8	−96.28 (17)	Zr1—O5—C11—C8	−19.8 (4)
O1—Zr1—N2—C8	83.72 (17)	N2—C8—C11—O6	−169.6 (3)
O5—Zr1—N2—C8	−7.83 (17)	C9—C8—C11—O6	11.1 (5)
O5^{i}—Zr1—N2—C8	172.17 (17)	N2—C8—C11—O5	10.4 (4)
N1^{i}—Zr1—N2—C8	−141.88 (17)	C9—C8—C11—O5	−168.9 (3)
N1—Zr1—N2—C8	38.12 (17)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*NA*···O1	0.77	2.23	3.003 (4)	175
N3—H3*NB*···O2*W*^{i}	0.86	2.15	2.930 (4)	150
N4—H4*NA*···O2*W*^{i}	0.83	2.04	2.818 (4)	156
N4—H4*NB*···O1*W*^{ii}	0.78	2.06	2.834 (4)	175
N5—H5*NA*···O2	0.88	1.95	2.828 (4)	171
N5—H5*NB*···O3^{iii}	0.79	2.45	3.143 (4)	148
N5—H5*NB*···O4^{iii}	0.79	2.52	3.171 (4)	141
O1*W*—H1*WA*···O3^{iv}	0.84	2.33	3.041 (3)	143
O1*W*—H1*WA*···O5^{iv}	0.84	2.38	3.076 (3)	140
O1*W*—H1*WB*···O6	0.89	1.87	2.761 (3)	175
O2*W*—H2*WA*···O5^{iv}	0.86	2.07	2.909 (3)	165
O2*W*—H2*WA*···O6^{iv}	0.86	2.57	3.085 (3)	119
O2*W*—H2*WB*···O4^{v}	0.94	1.84	2.745 (3)	160

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