metal-organic compounds

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catena-Poly[[zinc-µ-[2-(2-{[2-(2-hydroxybenzoyl)hydrazinylidene]methyl}phenoxy)acetato(2–)]] monohydrate]

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ (C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.109; data-to-parameter ratio = 13.6.

In the title compound, $\{[Zn(C_{16}H_{12}N_2O_5)]\cdot H_2O\}_n$, the unique Zn^{II} ion is coordinated in a distorted square-pyramidal environment by three O atoms and one N atom from a symmetry-unique ligand. A symmetry-related ligand provides an O atom from a carboxylate group to complete the coordination in the apical site and generate a one-dimensional polymer parallel to [010]. In addition to an intramolecular O- $H \cdots O$ hydrogen bond, intermolecular O- $H \cdots O$ and weak C- $H \cdots O$ hydrogen bonds are observed within the one-dimensional structure.

Related literature

For background information on zinc(II) carboxylate compounds, see: Suen *et al.* (2002). For general information on the structures of carboxylate and hydrazone compounds, see: Wu *et al.* (2007); Luo *et al.* (2010).



Experimental

Crvstal data

$\begin{split} & [\text{Zn}(\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_5)] \cdot \text{H}_2\text{O} \\ & M_r = 395.66 \\ & \text{Monoclinic, } P2_1/c \\ & a = 14.730 \ (2) \text{ Å} \\ & b = 5.4063 \ (8) \text{ Å} \\ & c = 20.983 \ (3) \text{ Å} \\ & \beta = 106.620 \ (2)^\circ \end{split}$	$V = 1601.2 \text{ (4) } \text{Å}^{3}$ Z = 4 Mo K\alpha radiation $\mu = 1.57 \text{ mm}^{-1}$ T = 298 K 0.16 \times 0.12 \times 0.10 mm
Data collection	
Bruker SMART CCD	3132 independent reflections
9785 measured reflections	$R_{\rm int} = 0.092$
Refinement	
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of
$wR(F^2) = 0.109$	independent and constrained
S = 1.06	refinement
3132 reflections	$\Delta \rho_{\rm max} = 0.48 \text{ e A}^{-3}$
230 parameters	$\Delta \rho_{\rm min} = -0.51 \text{ e A}^{-5}$

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdot \cdot \cdot A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$\begin{array}{l} O2 - H20 \cdots N1 \\ O6 - H60A \cdots O1^{i} \\ C8 - H8 \cdots O2^{ii} \end{array}$	0.75 (4)	1.92 (4)	2.583 (3)	148 (4)
	0.84	2.22	3.056 (4)	179
	0.93	2.41	3.316 (4)	164

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5346).

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catena-Poly[[zinc-µ-[2-(2-{[2-(2-hydroxybenzoyl)hydrazinylidene]methyl}phenoxy)acetato(2-)]] monohydrate]

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Comment

Zn(II) carboxylates, especially those with nitrogen donor ligands, have been the subject of numerous investigations (Suen *et al.*, 2002). Different coordination modes of carboxylate groups can form mononuclear and polynuclear structures. Hydrazone with carboxylate groups can also form mononuclear and polynuclear structures in different conditions (Wu *et al.*, 2007; Luo *et al.*, 2010). Herein we report the synthesis and crystal structure of the title compound.

Part of the one-dimensional structure is shown in Fig. 1. The unique Zn^{II} ion is coordinated in a distorted square-pyramidal environment by three O atoms and one N atom from a symmetry unique ligand. A symmetry related ligand provides an O atom from a carboxylate group to complete the coordination in the apical site and generate a one-dimensional polymer parallel to [010] (Fig 2). In addition to an intramolecular O—H···N hydrogen bond, intermolecular O—H···O and weak C—H···O hydrogen bonds are observed within the one

Experimental

The hydrazone ligand was synthesized according to the literature procedure (Luo *et al.*, 2010). Zinc(II) acetate monohydrate (1 mmol) was dissolved in methanol (15 ml), to which a solution of the ligand (2.5 mmol) in dimethylformamide (15 ml) was added. The mixture was stirred for 3 h at room temperature. An light-yellow solution was obtained, the solution was filtered and allowed to stand at room temperature for three weeks, where upon colorless block-shaped crystals were obtained.

Refinement

All H atoms, except for H2O were placed in idealized positions and allowed to ride on their parent atoms, with O—H = 0.84 Å (water), C—H = 0.93-0.97 Å and $U_{iso}=1.2-1.5 \text{ U}_{eq}(C,O)$. The hydroxy H atom (H2O) was refined independently with an isotropic displacement parameter.

Figures



Fig. 1. The molecular structure of with displacement ellipsoids drawn at the 30% probability level [symmetry codes: (a) -x+1, y-1/2, -z+1/2; (b) -x+1, y+1/2, -z+1/2]. H atoms are not shown.



catena-Poly[[zinc-µ-[2-(2-{[2-(2- hydroxybenzoyl)hydrazinylidene]methyl}phenoxy)acetato(2-)]] monohydrate]

Crystal data	
$[Zn(C_{16}H_{12}N_2O_5)]\cdot H_2O$	F(000) = 808
$M_r = 395.66$	$D_{\rm x} = 1.641 {\rm ~Mg~m^{-3}}$
Monoclinic, $P2_1/c$	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3978 reflections
a = 14.730 (2) Å	$\theta = 2.8-27.4^{\circ}$
b = 5.4063 (8) Å	$\mu = 1.57 \text{ mm}^{-1}$
c = 20.983 (3) Å	<i>T</i> = 298 K
$\beta = 106.620 \ (2)^{\circ}$	Block, colorless
V = 1601.2 (4) Å ³	$0.16 \times 0.12 \times 0.10 \text{ mm}$
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2764 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\rm int} = 0.092$
graphite	$\theta_{\text{max}} = 26.0^{\circ}, \ \theta_{\text{min}} = 2.0^{\circ}$
φ and ω scans	$h = -16 \rightarrow 18$
9785 measured reflections	$k = -6 \rightarrow 6$
3132 independent reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.109$	H atoms treated by a mixture of independent and constrained refinement
<i>S</i> = 1.06	$w = 1/[\sigma^2(F_0^2) + (0.0552P)^2 + 0.0104P]$ where $P = (F_0^2 + 2F_c^2)/3$
3132 reflections	$(\Delta/\sigma)_{\rm max} = 0.001$
230 parameters	$\Delta \rho_{max} = 0.48 \text{ e} \text{ Å}^{-3}$
0 restraints	$\Delta \rho_{\rm min} = -0.51 \text{ e } \text{\AA}^{-3}$

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.

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Zn1	0.37549 (2)	0.04095 (6)	0.273648 (16)	0.03342 (14)
O1	0.33632 (13)	-0.1912 (4)	0.33490 (10)	0.0408 (5)
O2	0.04795 (17)	-0.1639 (6)	0.32481 (16)	0.0713 (8)
O3	0.35695 (13)	0.1914 (4)	0.16947 (9)	0.0381 (5)
O4	0.45124 (12)	-0.1779 (3)	0.23378 (9)	0.0347 (4)
O5	0.54232 (13)	-0.2163 (4)	0.16671 (9)	0.0401 (5)
N1	0.18798 (16)	-0.0372 (4)	0.28074 (13)	0.0380 (6)
N2	0.23483 (15)	0.1069 (4)	0.24511 (11)	0.0320 (5)
C1	0.2011 (2)	-0.3599 (5)	0.35985 (14)	0.0396 (7)
C2	0.1069 (2)	-0.3391 (7)	0.35924 (17)	0.0522 (8)
C3	0.0705 (3)	-0.5039 (8)	0.3972 (2)	0.0722 (12)
H3	0.0084	-0.4860	0.3988	0.087*
C4	0.1252 (3)	-0.6905 (7)	0.43192 (19)	0.0711 (12)
H4	0.0998	-0.8000	0.4564	0.085*
C5	0.2174 (3)	-0.7179 (6)	0.43094 (17)	0.0624 (10)
H5	0.2541	-0.8471	0.4541	0.075*
C6	0.2553 (3)	-0.5528 (5)	0.39543 (16)	0.0475 (8)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A^2)

H6	0.3181	-0.5705	0.3952	0.057*
C7	0.24582 (19)	-0.1871 (5)	0.32341 (13)	0.0334 (6)
C8	0.1840 (2)	0.2634 (5)	0.20485 (14)	0.0402 (7)
H8	0.1218	0.2832	0.2061	0.048*
C9	0.2143 (2)	0.4136 (5)	0.15722 (14)	0.0364 (6)
C10	0.29665 (18)	0.3766 (5)	0.13731 (13)	0.0317 (6)
C11	0.3143 (2)	0.5182 (5)	0.08720 (15)	0.0384 (7)
H11	0.3689	0.4913	0.0743	0.046*
C12	0.2508 (2)	0.6998 (5)	0.05635 (15)	0.0460 (7)
H12	0.2627	0.7940	0.0225	0.055*
C13	0.1696 (2)	0.7423 (6)	0.07554 (16)	0.0536 (8)
H13	0.1275	0.8663	0.0552	0.064*
C14	0.1519 (2)	0.5995 (6)	0.12493 (17)	0.0516 (8)
H14	0.0969	0.6274	0.1372	0.062*
C15	0.42785 (19)	0.1002 (5)	0.14144 (14)	0.0343 (6)
H15A	0.4731	0.2296	0.1406	0.041*
H15B	0.3992	0.0441	0.0962	0.041*
C16	0.47695 (18)	-0.1127 (5)	0.18446 (13)	0.0332 (6)
O6	0.4589 (3)	0.7641 (10)	0.47903 (19)	0.171 (2)
H60A	0.4249	0.7787	0.4396	0.256*
H60B	0.5164	0.7397	0.4823	0.256*
H20	0.074 (3)	-0.090 (7)	0.305 (2)	0.067 (13)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0246 (2)	0.0419 (2)	0.0363 (2)	0.00089 (12)	0.01278 (15)	0.00451 (13)
01	0.0301 (10)	0.0488 (12)	0.0463 (12)	0.0011 (9)	0.0154 (9)	0.0140 (9)
O2	0.0348 (13)	0.093 (2)	0.094 (2)	-0.0094 (14)	0.0308 (14)	0.0222 (17)
O3	0.0306 (10)	0.0517 (12)	0.0363 (11)	0.0114 (9)	0.0163 (8)	0.0117 (9)
O4	0.0331 (10)	0.0378 (10)	0.0368 (10)	0.0055 (8)	0.0157 (8)	0.0039 (8)
O5	0.0315 (10)	0.0508 (11)	0.0411 (11)	0.0072 (9)	0.0153 (9)	0.0016 (9)
N1	0.0270 (12)	0.0492 (14)	0.0417 (14)	-0.0039 (10)	0.0160 (11)	0.0052 (11)
N2	0.0240 (11)	0.0389 (12)	0.0354 (13)	0.0020 (9)	0.0123 (10)	0.0045 (10)
C1	0.0453 (17)	0.0440 (16)	0.0323 (15)	-0.0146 (14)	0.0156 (13)	-0.0054 (12)
C2	0.0429 (18)	0.061 (2)	0.055 (2)	-0.0190 (17)	0.0189 (16)	0.0034 (17)
C3	0.067 (3)	0.085 (3)	0.076 (3)	-0.038 (2)	0.038 (2)	-0.004 (2)
C4	0.100 (3)	0.064 (2)	0.058 (2)	-0.043 (2)	0.037 (2)	-0.0004 (19)
C5	0.093 (3)	0.052 (2)	0.0418 (19)	-0.019 (2)	0.0199 (19)	0.0033 (15)
C6	0.059 (2)	0.0452 (17)	0.0401 (18)	-0.0089 (15)	0.0163 (16)	-0.0020 (13)
C7	0.0319 (14)	0.0365 (14)	0.0339 (14)	-0.0066 (11)	0.0130 (12)	-0.0046 (11)
C8	0.0257 (14)	0.0531 (17)	0.0448 (17)	0.0032 (12)	0.0147 (13)	0.0049 (14)
C9	0.0345 (15)	0.0409 (15)	0.0342 (15)	0.0071 (12)	0.0104 (12)	0.0046 (12)
C10	0.0282 (13)	0.0345 (13)	0.0308 (14)	0.0006 (11)	0.0056 (11)	-0.0004 (11)
C11	0.0381 (16)	0.0416 (15)	0.0359 (16)	-0.0031 (12)	0.0112 (13)	0.0004 (12)
C12	0.057 (2)	0.0418 (16)	0.0381 (16)	-0.0013 (14)	0.0127 (15)	0.0060 (13)
C13	0.063 (2)	0.0492 (18)	0.0487 (19)	0.0229 (16)	0.0155 (17)	0.0140 (15)
C14	0.0488 (19)	0.0548 (19)	0.055 (2)	0.0195 (16)	0.0202 (16)	0.0116 (16)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15	0.0279 (14)	0.0438 (15)	0.0337 (15)	0.0032 (12)	0.0127 (12)	0.0008 (12)
06 0.097 (3) 0.327 (7) 0.087 (3) -0.054 (4) 0.023 (2) -0.067 (4) Geometric parameters (Å, °) Zan I04 1.9694 (17) C4C5 1.372 (6) Zan I05 ^d 1.9717 (19) C4H4 0.9300 Zan I01 1.9958 (18) C5C6 1.379 (4) Zan I-03 2.2743 (18) C6H6 0.9300 $01-C7$ 1.285 (3) C8C9 1.454 (4) $02L12$ 0.3301 C9C14 1.400 (4) $03C10$ 1.380 (3) C9C10 1.406 (4) $03C16$ 1.259 (3) C11C12 1.382 (4) $04C16$ 1.259 (3) C11H11 0.9300 $05Zn1^{ti}$ 1.322 (4) C12C13 1.387 (4) $NI-C7$ 1.322 (4) C13H13 0.9300 $05Za1^{ti}$ 1.376 (4) C13H13 0.9300 $C1-C2$ 1.389 (4) C14H14 0.9300 $C1-C3$ 1.389 (4) C15C16 1.513 (C16	0.0275 (14)	0.0370 (14)	0.0354 (15)	-0.0026 (11)	0.0094 (12)	-0.0041 (12)
Geometric parameters (Å, 9) Zn1-O4 19694 (17) C4-C5 1.372 (6) Zn1-O5 ⁱ 1.9717 (19) C4-H4 0.9300 Zn1-O1 1.9958 (18) C5-C6 1.379 (4) Zn1-O3 2.2743 (18) C6-H6 0.9300 Ol-C7 1.285 (3) C8-C9 1.454 (4) O2-C2 1.347 (4) C8-H8 0.9300 O2-H20 0.75 (4) C9-C14 1.400 (4) O3-C15 1.425 (3) C10-C11 1.382 (4) O3-C16 1.250 (3) C11-C12 1.382 (4) O5-C16 1.259 (3) C11-H11 0.9300 O5-Zn1 ⁱⁱ 1.9717 (19) C12-C13 1.387 (4) N1-C7 1.322 (4) C12-H12 0.9300 N1-N2 1.392 (3) C13-H13 0.9300 C1-C2 1.389 (4) C14-H14 0.9300 C1-C2 1.389 (4) C14-H14 0.9300 C1-C2 1.389 (4) C15-H15A 0.9700 C1-C2 1.389 (4) C15-H14 0.9300 C1-C2 1.389 (4) C	O6	0.097 (3)	0.327 (7)	0.087 (3)	-0.054 (4)	0.023 (2)	-0.067 (4)
Zn1O41.9694 (17)C4C51.372 (6)Zn1O5 ⁱ 1.9717 (19)C4H40.9300Zn1-O11.9958 (18)C5C61.379 (4)Zn1-N22.017 (2)C5H50.9300O1C71.285 (3)C6H60.9300O1C71.285 (3)C8C91.454 (4)O2C21.347 (4)C8H80.9300O2-H200.75 (4)C9C141.400 (4)O3C101.380 (3)C9C101.406 (4)O3C151.425 (3)C10C111.385 (4)O4C161.259 (3)C11C121.382 (4)O5Zn1 ¹¹ 1.9717 (19)C12C131.387 (4)NI-C71.332 (4)C12H110.9300O5-Zn1 ¹¹ 1.9717 (19)C12-C141.306 (4)N1-C71.332 (4)C13H130.9300C1-C21.389 (4)C13H130.9300C1-C21.389 (4)C15H130.9300C1-C41.392 (3)C13H130.9300C1-C51.393 (4)C15H161.513 (4)C2-C31.400 (5)C15H15A0.9700C3-C41.365 (6)06-H60A0.8400C3-L1-O5 ¹ 110.48 (8)C5C6-H6119.5C4-Zn1-O5 ¹ 101.48 (8)C1C7-N1124.8 (2)O4-Zn1-O5 ¹ 101.48 (8)C1C6-H6119.5C3 ¹ -Zn1-O1101.48 (8)C1C6-H6119.5C3 ¹ -Zn1-O37.454 (7)N2C8C9126.0 (2)O4-Zn1-O37.454 (7)	Geometric pa	arameters (Å, °)					
$Zn1-OS^i$ 1.9717 (19) $C4-H4$ 0.9300 $Zn1-O1$ 1.9958 (18) $C5-C6$ 1.379 (4) $Zn1-N2$ 2.017 (2) $C5-H5$ 0.9300 $Zn1-O3$ 2.2743 (18) $C6-H6$ 0.9300 $O1-C7$ 1.285 (3) $C8-C9$ 1.454 (4) $O2-C2$ 1.347 (4) $C8-H8$ 0.9300 $O2-H20$ 0.75 (4) $C9-C14$ 1.406 (4) $O3-C10$ 1.380 (3) $C9-C10$ 1.485 (4) $O3-C15$ 1.425 (3) $C10-C11$ 1.385 (4) $O4-C16$ 1.259 (3) $C11-C12$ 1.387 (4) $O5-C16$ 1.259 (3) $C11-C12$ 1.387 (4) $O5-Zn1^{10}$ 1.9717 (19) $C12-C13$ 1.387 (4) $N1-C7$ 1.322 (4) $C12-H12$ 0.9300 $O5-Zn1^{10}$ 1.392 (3) $C13-C14$ 1.376 (4) $N2-C8$ 1.276 (3) $C13-H13$ 0.9300 $C1-C6$ 1.393 (4) $C15-C16$ 1.513 (4) $C1-C7$ 1.476 (4) $C15-H15A$ 0.9700 $C2-C3$ 1.400 (5) $C15-H15A$ 0.9700 $C3-C4$ 1.365 (6) $O6-H60A$ 0.8400 $O4-Zn1-O1$ 101.48 (8) $C1-C6-H6$ 119.5 $O4-Zn1-O3$ 79.67 (8) $C1-C7-N1$ 1.424.8 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 79.67 (8) $C1-C6-H6$ 119.5 (3) $O4-Zn1-O3$ 79.67 (8) $C1-C6-H6$ 119.5 (3) $O4-Zn1-O3$ 79.67 (8) $C1-C6-C9-C8$ 116.5 (3) $O4-Zn1-O3$ 104.79 (7)<	Zn1—O4		1.9694 (17)	C4—	C5	1.3	72 (6)
Zn1-O11.9958 (18)C5-C61.379 (4)Zn1-N22.017 (2)C5-H50.9300Zn1-O32.2743 (18)C6-H60.9300O1-C71.285 (3)C8-C91.454 (4)02-C21.347 (4)C8-H80.930002-H200.75 (4)C9-C141.400 (4)03-C101.380 (3)C9-C101.466 (4)03-C151.425 (3)C10-C111.385 (4)04-C161.250 (3)C11-C121.382 (4)05-C161.259 (3)C12-C131.387 (4)N1-C71.322 (4)C12-C131.387 (4)N1-C71.322 (4)C12-C141.376 (4)N2-C81.276 (3)C13-C141.376 (4)N2-C81.276 (3)C13-H130.9300C1-C21.389 (4)C15-C161.513 (4)C1-C71.476 (4)C15-H15A0.9700C2-C31.400 (5)C15-H15B0.9700C3-C41.365 (6)O6-H60A0.8400C3-H30.9300O6-H60B0.8400C4-Zn1-O1101.48 (8)C1-C6-H6119.5O4-Zn1-O1104.85 (8)N2-C8-O9126.0 (2)O4-Zn1-N280.84 (8)N2-C8-C9126.0 (2)O4-Zn1-N210.948 (8)N2-C8-C9126.0 (2)O4-Zn1-N280.84 (8)N2-C8-C9126.0 (2)O4-Zn1-N210.47 (7)N2-C8-H8117.0O5-Zn1-N210.47 (7)N2-C8-H8117.0O1-Zn1-N280.84 (8)N2-C8-C9126.0 (2) <td< td=""><td>Zn1—O5ⁱ</td><td></td><td>1.9717 (19)</td><td>C4—</td><td>H4</td><td>0.93</td><td>300</td></td<>	Zn1—O5 ⁱ		1.9717 (19)	C4—	H4	0.93	300
Zn1-N22.017 (2)C5-H50.9300Zn1-O32.2743 (18)C6-H60.9300O1-C71.285 (3)C8-C91.454 (4)O2-C21.347 (4)C8-H80.9300O2-H200.75 (4)C9-C141.400 (4)O3-C101.380 (3)C9-C101.406 (4)O3-C151.425 (3)C10-C111.385 (4)O4-C161.250 (3)C11-H10.9300O5-C161.259 (3)C11-H110.9300O5-Zn1 ⁱⁱ 1.9717 (19)C12-C131.387 (4)N1-C71.322 (4)C12-H120.9300N1-N21.392 (3)C13-C141.376 (4)N2-C81.276 (3)C13-H130.9300C1-C21.389 (4)C14-H140.9300C1-C61.393 (4)C15-C161.513 (4)C1-C74.476 (4)C15-H15B0.9700C2-C31.400 (5)C15-H15B0.9700C3-C41.365 (6)0.6-H60A0.8400C3-H30.930006-H60B0.8400C4-Zn1-O1101.48 (8)C1-C6-H6119.5O4-Zn1-O374.54 (7)N2-C8-C9126.0 (2)O4-Zn1-N2129.69 (9)01-C7-N1124.8 (2)O4-Zn1-O374.54 (7)N2-C8-H8117.0O1-Zn1-N280.84 (8)N2-C8-C9126.0 (2)O4-Zn1-O374.54 (7)N2-C8-H8117.0O1-Zn1-O3150.04 (8)C14-C9-C10117.5 (3)N2-Zn1-O379.67 (8)C14-C9-C816.5 (3)C7-	Zn1—O1		1.9958 (18)	С5—	C6	1.3	79 (4)
Zn1-O32.2743 (18)C6-H60.9300 $O1-C7$ 1.285 (3)CR-C91.454 (4) $O2-C2$ 1.347 (4)C8-H80.9300 $O2-H20$ 0.75 (4)C9-C141.400 (4) $O3-C10$ 1.380 (3)C9-C101.406 (4) $O3-C15$ 1.425 (3)C10-C111.385 (4) $O4-C16$ 1.250 (3)C11-C121.382 (4) $O5-C16$ 1.259 (3)C11-H110.9300 $O5-Zn1^{ii}$ 1.9717 (19)C12-C131.387 (4) $NI-C7$ 1.322 (4)C12-H120.9300 $NI-N2$ 1.392 (3)C13-C141.376 (4) $N2-C8$ 1.276 (3)C13-H130.9300C1-C21.389 (4)C14-H140.9300C1-C41.376 (4)C15-C161.513 (4)C1-C71.476 (4)C15-H15A0.9700C2-C31.400 (5)C15-H15A0.9700C3-C41.365 (6)O6-H60A0.8400C3-H30.9300O6-H60B0.8400C4-Zn1-O1104.88 (8)C5-C6-H6119.5O5'-Zn1-O1104.85 (8)O1-C7-N1124.8 (2)O4-Zn1-O2126.96 (9)01-C7-C1119.0 (2)O5'-Zn1-N219.04 (8)C1-C6-H6119.5O5'-Zn1-N210.448 (8)N2-C8-C9126.0 (2)O4-Zn1-O374.54 (7)N2-C8-H8117.0O1-Zn1-O3150.04 (8)C14-C9-C8165 (3)C7-O1-Zn1110.12 (16)C10-C9-C8125.9 (2)C2-O2-H20109 (3)03-C10-C1	Zn1—N2		2.017 (2)	С5—	Н5	0.93	300
$01-C7$ 1.285 (3) $C8-C9$ 1.454 (4) $02-C2$ 1.347 (4) $C8-H8$ 0.9300 $02-H20$ 0.75 (4) $C9-C14$ 1.400 (4) $03-C10$ 1.380 (3) $C9-C10$ 1.406 (4) $03-C15$ 1.425 (3) $C10-C11$ 1.385 (4) $04-C16$ 1.250 (3) $C11-C12$ 1.382 (4) $05-C16$ 1.259 (3) $C11-H11$ 0.9300 $O5-Zn1^{II}$ 1.9717 (19) $C12-C13$ 1.387 (4) $N1-C7$ 1.322 (4) $C12-H12$ 0.9300 $N-N2$ 1.392 (3) $C13-C14$ 1.376 (4) $N2-C8$ 1.276 (3) $C13-H13$ 0.9300 $C1-C2$ 1.389 (4) $C14-H14$ 0.9300 $C1-C6$ 1.393 (4) $C15-C16$ 1.513 (4) $C1-C7$ 1.476 (4) $C15-H15A$ 0.9700 $C2-C3$ 1.400 (5) $C15-H15B$ 0.9700 $C3-C4$ 1.365 (6) $O6-H60A$ 0.8400 $C4-Zn1-O1$ 101.48 (8) $C1-C7-N1$ 124.8 (2) $O4-Zn1-O1$ 104.35 (8) $O1-C7-C1$ 119.0 (2) $Os^i-Zn1-N2$ 17.57 (9) $N1-C7-C1$ 119.0 (2) $Os^i-Zn1-N2$ 17.57 (9) $N1-C7-C1$ 119.0 (2) $Os^i-Zn1-N2$ 104.79 (7) $C9-C8-H8$ 117.0 $O1-Zn1-O3$ 74.54 (7) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 79.67 (8) $C14-C9-C10$ 117.5 (3) $O2-Zn1-O3$ 79.67 (8) $C14-C9-C10$ 117.5 (3) $O2-Zn1-O3$ 79.67 (8) $C14-C9-C8$ 125.9 (2) $O2-Zn1-O3$	Zn1—O3		2.2743 (18)	С6—	Н6	0.93	300
$02-C2$ 1.347 (4) $C8-H8$ 0.9300 $02-H20$ 0.75 (4) $C9-C14$ 1.400 (4) $03-C10$ 1.380 (3) $C9-C10$ 1.406 (4) $03-C15$ 1.425 (3) $C10-C11$ 1.385 (4) $04-C16$ 1.259 (3) $C11-C12$ 1.382 (4) $05-C16$ 1.259 (3) $C11-H11$ 0.9300 $05-Zn1^{H}$ 1.9717 (19) $C12-C13$ 1.387 (4) $N1-C7$ 1.322 (4) $C12-H12$ 0.9300 $N-N2$ 1.392 (3) $C13-C14$ 1.376 (4) $N2-C8$ 1.276 (3) $C13-H13$ 0.9300 $C1-C2$ 1.389 (4) $C14-H14$ 0.9300 $C1-C6$ 1.393 (4) $C15-C16$ 1.513 (4) $C1-C7$ 1.476 (4) $C15-H15A$ 0.9700 $C2-C3$ 1.400 (5) $C15-H15B$ 0.9700 $C3-C4$ 1.365 (6) $06-H60B$ 0.8400 $C3-H3$ 0.9300 $O6-H60B$ 0.8400 $O4-Zn1-O5^i$ 110.48 (8) $C5-C6-H6$ 119.5 $O5^i-Zn1-O1$ 104.35 (8) $O1-C7-N1$ 124.8 (2) $O4-Zn1-N2$ 129.69 (9) $O1-C7-C1$ 116.3 (2) $O1-Zn1-N2$ 80.84 (8) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O5^i-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.5 (3) $O2-C0-H20$ 109 (3) $O3-C10-C11$ 122.6 (2) $(1-O-O)-Zn1$ 110.12 (16) $C10-C9-C8$ 125.9 (2) $(2$	O1—C7		1.285 (3)	C8—	С9	1.4:	54 (4)
$02-H20$ 0.75 (4) $C9-C14$ 1.400 (4) $03-C10$ 1.380 (3) $C9-C10$ 1.406 (4) $03-C15$ 1.425 (3) $C10-C11$ 1.385 (4) $04-C16$ 1.250 (3) $C11-C12$ 1.382 (4) $05-C16$ 1.259 (3) $C11-H11$ 0.9300 $05-Zn1^{11}$ 1.9717 (19) $C12-C13$ 1.387 (4) $N1-C7$ 1.322 (4) $C12-H12$ 0.9300 $N-N2$ 1.392 (3) $C13-C14$ 1.376 (4) $N2-C8$ 1.276 (3) $C13-H13$ 0.9300 $C1-C2$ 1.389 (4) $C14-H14$ 0.9300 $C1-C6$ 1.393 (4) $C15-C16$ 1.513 (4) $C1-C7$ 1.476 (4) $C15-H15A$ 0.9700 $C2-C3$ 1.400 (5) $C15-H15B$ 0.9700 $C3-C4$ 1.365 (6) $06-H60A$ 0.8400 $C4-Zn1-O5^i$ 110.48 (8) $C5-C6-H6$ 119.5 $O4-Zn1-O5^i$ 10.48 (8) $C5-C6-H6$ 119.5 $O5^1-Zn1-O1$ 104.35 (8) $01-C7-N1$ 124.8 (2) $O4-Zn1-N2$ 129.69 (9) $01-C7-C1$ 116.3 (2) $O1-Zn1-N2$ 80.84 (8) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-C8$ 117.5 (3) $O2-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O5^1-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.5 (3) $O2-Zn1-O3$ 79.67 (8) $C14-C9-C10$ 117.5 (3) $O2-Zn1-O3$ 79.67 (8) $C14-C9-C10$ 117.5 (3)	O2—C2		1.347 (4)	C8—	H8	0.93	300
$03-C10$ $1.380 (3)$ $C9-C10$ $1.406 (4)$ $03-C15$ $1.425 (3)$ $C10-C11$ $1.385 (4)$ $04-C16$ $1.250 (3)$ $C11-C12$ $1.382 (4)$ $05-C16$ $1.259 (3)$ $C11-H11$ 0.9300 $05-Zn1^{ii}$ $1.9717 (19)$ $C12-C13$ $1.387 (4)$ $N1-C7$ $1.322 (4)$ $C12-H12$ 0.9300 $N1-N2$ $1.392 (3)$ $C13-C14$ 0.9300 $N-C4$ $1.376 (4)$ 0.9300 $N-C2$ $1.389 (4)$ $C14-H14$ 0.9300 $C1-C2$ $1.389 (4)$ $C15-C16$ $1.513 (4)$ $C1-C6$ $1.393 (4)$ $C15-H15A$ 0.9700 $C2-C3$ $1.400 (5)$ $C15-H15A$ 0.9700 $C2-C3$ $1.400 (5)$ $C15-H15B$ 0.9700 $C3-C4$ $1.365 (6)$ $06-H60A$ 0.8400 $C3-H3$ 0.9300 $06-H60B$ 0.8400 $O4-Zn1-O5^{i}$ $110.48 (8)$ $C5-C6-H6$ 119.5 $O4-Zn1-O1$ $101.48 (8)$ $C1-C6-H6$ 119.5 $O5^{i}-Zn1-O1$ $104.35 (8)$ $O1-C7-N1$ $124.8 (2)$ $O4-Zn1-N2$ $80.84 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $74.54 (7)$ $N2-C8-H8$ 117.0 $O5^{i}-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $79.67 (8)$ $C14-C9-C10$ $117.5 (3)$ $N2-Zn1-O3$ $79.67 (8)$ $C14-C9-C8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 $	O2—H20		0.75 (4)	С9—	C14	1.40	00 (4)
$03-C15$ $1.425 (3)$ $C10-C11$ $1.385 (4)$ $04-C16$ $1.250 (3)$ $C11-C12$ $1.382 (4)$ $05-C16$ $1.259 (3)$ $C11-H11$ 0.9300 $05-Zn1^{ii}$ $1.9717 (19)$ $C12-C13$ $1.387 (4)$ $N1-C7$ $1.322 (4)$ $C12-H12$ 0.9300 $N1-N2$ $1.392 (3)$ $C13-C14$ $1.376 (4)$ $N2-C8$ $1.276 (3)$ $C13-H13$ 0.9300 $C1-C2$ $1.389 (4)$ $C14-H14$ 0.9300 $C1-C6$ $1.393 (4)$ $C15-C16$ $1.513 (4)$ $C1-C7$ $1.476 (4)$ $C15-H15A$ 0.9700 $C2-C3$ $1.400 (5)$ $C15-H15B$ 0.9700 $C3-C4$ $1.365 (6)$ $06-H60A$ 0.8400 $C3-C4$ $1.365 (6)$ $06-H60B$ 0.8400 $C4-Zn1-O5^i$ $110.48 (8)$ $C1-C6-H6$ 119.5 $O4-Zn1-O1$ $101.48 (8)$ $C1-C6-H6$ 119.5 $O5^i-Zn1-N2$ $17.57 (9)$ $N1-C7-C1$ $116.3 (2)$ $O1-Zn1-N2$ $80.84 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $74.54 (7)$ $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.97 (7)$ $C9-C8-H8$ $115.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C14-C9-C10$ $117.5 (3)$ $N2-Zn1-O3$ $79.67 (8)$ $C14-C9-C8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 (3)$ $O3-C10-C11$ $122.6 (2)$ </td <td>O3—C10</td> <td></td> <td>1.380 (3)</td> <td>С9—</td> <td>C10</td> <td>1.40</td> <td>06 (4)</td>	O3—C10		1.380 (3)	С9—	C10	1.40	06 (4)
$04-C16$ $1.250 (3)$ $C11-C12$ $1.382 (4)$ $05-C16$ $1.259 (3)$ $C11-H11$ 0.9300 $05-Zn1^{ii}$ $1.9717 (19)$ $C12-C13$ $1.387 (4)$ $N1-C7$ $1.322 (4)$ $C12-H12$ 0.9300 $N1-N2$ $1.392 (3)$ $C13-C14$ $1.376 (4)$ $N2-C8$ $1.276 (3)$ $C13-H13$ 0.9300 $C1-C2$ $1.389 (4)$ $C14-H14$ 0.9300 $C1-C6$ $1.393 (4)$ $C15-C16$ $1.513 (4)$ $C1-C7$ $1.476 (4)$ $C15-H15A$ 0.9700 $C2-C3$ $1.400 (5)$ $C15-H15B$ 0.9700 $C3-C4$ $1.365 (6)$ $06-H60A$ 0.8400 $C3-H3$ 0.9300 $06-H60B$ 0.8400 $O4-Zn1-O5^i$ $110.48 (8)$ $C5-C6-H6$ 119.5 $O4-Zn1-O1$ $101.48 (8)$ $C1-C6-H6$ 119.5 $O5^i-Zn1-O1$ $104.35 (8)$ $01-C7-N1$ $124.8 (2)$ $O4-Zn1-N2$ $12.969 (9)$ $01-C7-C1$ $116.3 (2)$ $O5^i-Zn1-N2$ $117.57 (9)$ $N1-C7-C1$ $116.3 (2)$ $O1-Zn1-N2$ $80.84 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $104.79 (7)$ $O2-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 (3)$ $O3-C10-C11$ $122.6 (2)$ $C10-O3-C15$ $119.63 (19)$ $O3-C10-C9$ $16.6(2)$	O3—C15		1.425 (3)	C10–	C11	1.38	35 (4)
$05-C16$ 1.259 (3) $C11-H11$ 0.9300 $05-Zn1^{ji}$ 1.9717 (19) $C12-C13$ 1.387 (4) $N1-C7$ 1.322 (4) $C12-H12$ 0.9300 $N1-N2$ 1.392 (3) $C13-C14$ 1.376 (4) $N2-C8$ 1.276 (3) $C13-H13$ 0.9300 $C1-C2$ 1.389 (4) $C14-H14$ 0.9300 $C1-C4$ 1.376 (4) $C15-C16$ 1.513 (4) $C1-C6$ 1.393 (4) $C15-C16$ 1.513 (4) $C1-C7$ 1.476 (4) $C15-H15A$ 0.9700 $C2-C3$ 1.400 (5) $C15-H15B$ 0.9700 $C3-C4$ 1.365 (6) $06-H60A$ 0.8400 $C3-C4$ 1.365 (6) $06-H60B$ 0.8400 $C4-Zn1-O5^i$ 110.48 (8) $C5-C6-H6$ 119.5 $O4-Zn1-O1$ 101.48 (8) $C1-C7-N1$ 124.8 (2) $O4-Zn1-N2$ 129.69 (9) $O1-C7-C1$ 119.0 (2) $O5^i-Zn1-N2$ 117.57 (9) $N1-C7-C1$ 116.3 (2) $O1-Zn1-N2$ 80.84 (8) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-H8$ 117.0 $O1-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O1-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $109.(3)$ $O3-C10-C9$ 125.9 (2) $C2-O2-H20$ 109 (3) $O3-C10-C9$ 125.9 (2) $C1-O2-C11$ 110.12 (16) $C10-C9-C8$ 125.9 (2) $C2-O2-H20$ 109 (3) $O3-C10-C9$ 16.6 (2) <td>O4—C16</td> <td></td> <td>1.250 (3)</td> <td>C11–</td> <td>C12</td> <td>1.38</td> <td>32 (4)</td>	O4—C16		1.250 (3)	C11–	C12	1.38	32 (4)
$O5-zn1^{ii}$ $1.9717 (19)$ $C12-C13$ $1.387 (4)$ $N1-C7$ $1.322 (4)$ $C12-H12$ 0.9300 $N1-N2$ $1.392 (3)$ $C13-C14$ $1.376 (4)$ $N2-C8$ $1.276 (3)$ $C13-H13$ 0.9300 $C1-C2$ $1.389 (4)$ $C14-H14$ 0.9300 $C1-C6$ $1.393 (4)$ $C15-C16$ $1.513 (4)$ $C1-C7$ $1.476 (4)$ $C15-H15A$ 0.9700 $C2-C3$ $1.400 (5)$ $C15-H15B$ 0.9700 $C3-C4$ $1.365 (6)$ $O6-H60A$ 0.8400 $C3-H3$ 0.9300 $O6-H60B$ 0.8400 $C4-Zn1-O5^i$ $110.48 (8)$ $C5-C6-H6$ 119.5 $O4-Zn1-O1$ $101.48 (8)$ $C1-C7-N1$ $124.8 (2)$ $O4-Zn1-N2$ $129.69 (9)$ $O1-C7-C1$ $116.3 (2)$ $O1-Zn1-N2$ $104.35 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $104.93 (8)$ $C14-C9-C10$ $117.5 (3)$ $N2-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 (3)$ $O3-C10-C11$ $122.6 (2)$ $C1-O3-C15$ $119.63 (19)$ $O3-C10-C9$ $116.6 (2)$	O5—C16		1.259 (3)	C11–	-H11	0.92	300
N1C7 $1.322 (4)$ C12H12 0.9300 N1N2 $1.392 (3)$ C13C14 $1.376 (4)$ N2C8 $1.276 (3)$ C13H13 0.9300 C1C2 $1.389 (4)$ C14H14 0.9300 C1C6 $1.393 (4)$ C15C16 $1.513 (4)$ C1C7 $1.476 (4)$ C15H15A 0.9700 C2C3 $1.400 (5)$ C15H15B 0.9700 C3C4 $1.365 (6)$ 06 H60A 0.8400 C3H3 0.9300 06 H60B 0.8400 C4Zn1O5 ⁱ $110.48 (8)$ C5C6H6 119.5 O4Zn1O1 $101.48 (8)$ C1C7N1 $124.8 (2)$ O4Zn1-N2 $129.69 (9)$ 01 C7C1 $119.0 (2)$ O5 ⁱ -Zn1-N2 $117.57 (9)$ $N1$ C7C1 $116.3 (2)$ O1Zn1-N2 $80.84 (8)$ $N2$ C8C9 $126.0 (2)$ O4Zn1-O3 $104.79 (7)$ C9C8H8 117.0 O1-Zn1-O3 $104.79 (7)$ C9C8H8 117.0 O1Zn1-O3 $190.04 (8)$ C14C9C10 $117.5 (3)$ N2Zn1-O3 $190.61 (8)$ $C14$ C9C8 $125.9 (2)$ C2-O2-H20 $109 (3)$ $O3$ C10C11 $122.6 (2)$ C10-O3C15 $119.63 (19)$ $O3$ C10C11 $122.6 (2)$ C10-O3C15 $119.63 (19)$ $O3$ C10C11 $122.6 (2)$	O5—Zn1 ⁱⁱ		1.9717 (19)	C12-	C13	1.38	37 (4)
N1-N21.392 (3)C13-C141.376 (4)N2-C81.276 (3)C13-H130.9300C1-C21.389 (4)C14-H140.9300C1-C61.393 (4)C15-C161.513 (4)C1-C71.476 (4)C15-H15A0.9700C2-C31.400 (5)C15-H15B0.9700C3-C41.365 (6)O6-H60A0.8400C3-H30.9300O6-H60B0.8400C4-Zn1-O5 ⁱ 110.48 (8)C5-C6-H6119.5O4-Zn1-O1101.48 (8)C1-C6-H6119.5O5 ⁱ -Zn1-O1104.35 (8)O1-C7-N1124.8 (2)O4-Zn1-N2129.69 (9)O1-C7-C1119.0 (2)O5 ⁱ -Zn1-N2117.57 (9)N1-C7-C1116.3 (2)O1-Zn1-N280.84 (8)N2-C8-C9126.0 (2)O4-Zn1-O374.54 (7)N2-C8-H8117.0O1-Zn1-O3150.04 (8)C14-C9-C10117.5 (3)N2-Zn1-O379.67 (8)C14-C9-C8116.5 (3)C7-O1-Zn1110.12 (16)C10-C9-C8125.9 (2)C2-O2-H20109 (3)O3-C10-C11122.6 (2)C10-O3-C15119.63 (19)O3-C10-C9116.6 (2)	N1—C7		1.322 (4)	C12–	-H12	0.93	300
N2-C81.276 (3)C13-H130.9300C1-C21.389 (4)C14-H140.9300C1-C61.393 (4)C15-C161.513 (4)C1-C71.476 (4)C15-H15A0.9700C2-C31.400 (5)C15-H15B0.9700C3-C41.365 (6)O6-H60A0.8400C3-H30.9300O6-H60B0.8400O4-Zn1-O5 ⁱ 110.48 (8)C5-C6-H6119.5O4-Zn1-O1101.48 (8)C1-C6-H6119.5O4-Zn1-N2129.69 (9)O1-C7-N1124.8 (2)O4-Zn1-N2117.57 (9)N1-C7-C1116.3 (2)O1-Zn1-N280.84 (8)N2-C8-C9126.0 (2)O4-Zn1-O374.54 (7)N2-C8-H8117.0O5 ⁱ -Zn1-O3104.79 (7)C9-C8-H8117.0O1-Zn1-O379.67 (8)C14-C9-C8125.9 (2)C2-C0-H20109 (3)O3-C10-C11122.6 (2)C10-O3-C15119.63 (19)O3-C10-C9116.6 (2)	N1—N2		1.392 (3)	C13–	C14	1.3	76 (4)
C1-C2 $1.389(4)$ C14-H14 0.9300 C1-C6 $1.393(4)$ C15-C16 $1.513(4)$ C1-C7 $1.476(4)$ C15-H15A 0.9700 C2-C3 $1.400(5)$ C15-H15B 0.9700 C3-C4 $1.365(6)$ 06 -H60A 0.8400 C3-H3 0.9300 06 -H60B 0.8400 C4-Zn1-O5 ⁱ $110.48(8)$ C5-C6-H6 119.5 C4-Zn1-O1 $101.48(8)$ C1-C6-H6 119.5 C4-Zn1-O1 $101.48(8)$ $C1$ -C7-N1 $124.8(2)$ C4-Zn1-N2 $129.69(9)$ 01 -C7-C1 $116.3(2)$ C4-Zn1-N2 $117.57(9)$ $N1$ -C7-C1 $116.3(2)$ C1-Zn1-N2 $80.84(8)$ $N2$ -C8-C9 $126.0(2)$ C4-Zn1-O3 $74.54(7)$ $N2$ -C8-H8 117.0 C5 ⁱ -Zn1-O3 $104.79(7)$ C9-C8-H8 117.0 C5 ⁱ -Zn1-O3 $19.67(8)$ C14-C9-C10 $117.5(3)$ N2-Zn1-O3 $79.67(8)$ C14-C9-C8 $125.9(2)$ C2-C0-H20 $109(3)$ $O3$ -C10-C11 $122.6(2)$ C10-O3-C15 $119.63(19)$ $O3$ -C10-C9 $120.0(2)$	N2—C8		1.276 (3)	C13–	-H13	0.93	300
C1C6 $1.393 (4)$ C15C16 $1.513 (4)$ C1C7 $1.476 (4)$ C15H15A 0.9700 C2C3 $1.400 (5)$ C15H15B 0.9700 C3C4 $1.365 (6)$ 06 H60A 0.8400 C3H3 0.9300 06 H60B 0.8400 C4Zn1O5 ⁱ 110.48 (8)C5C6H6119.5C4Zn1O1101.48 (8)C1C6H6119.5O4Zn1O1104.35 (8)O1C7N1124.8 (2)O4Zn1-N2129.69 (9)O1C7C1119.0 (2)O5 ⁱ Zn1-N2117.57 (9)N1C7C1116.3 (2)O1Zn1-N280.84 (8)N2C8C9126.0 (2)O4Zn1-O374.54 (7)N2C8H8117.0O5 ⁱ Zn1-O3150.04 (8)C14C9C10117.5 (3)N2Zn1-O379.67 (8)C14C9C8116.5 (3)C7O1Zn1110.12 (16)C10C9C8125.9 (2)C2O2H20109 (3)O3C10C11122.6 (2)C10O3C15119.63 (19)O3C10C9116.6 (2)	C1—C2		1.389 (4)	C14-	-H14	0.93	300
C1C71.476 (4)C15H15A0.9700C2C31.400 (5)C15H15B0.9700C3C41.365 (6)06H60A0.8400C3H30.930006H60B0.8400O4Zn1O5 ⁱ 110.48 (8)C5C6H6119.5O4Zn1O1101.48 (8)C1C6H6119.5O5 ⁱ Zn1O1104.35 (8)01C7N1124.8 (2)O4Zn1-N2129.69 (9)O1C7C1119.0 (2)O5 ⁱ Zn1-N2117.57 (9)N1C7C1116.3 (2)O1Zn1-N280.84 (8)N2C8C9126.0 (2)O4Zn1-O374.54 (7)N2C8H8117.0O5 ⁱ Zn1-O3104.79 (7)C9C8H8117.0O1Zn1-O3150.04 (8)C14C9C10117.5 (3)N2Zn1-O379.67 (8)C14C9C8116.5 (3)C7O1Zn1110.12 (16)C10-C9C8125.9 (2)C2O2H20109 (3)O3C10C11122.6 (2)C10O3C15119.63 (19)O3C10C9116.6 (2)C10-O3C15119.63 (15)C14C9C10116.6 (2)	C1—C6		1.393 (4)	C15-	C16	1.5	13 (4)
C2—C31.400 (5)C15—H15B0.9700C3—C41.365 (6)O6—H60A0.8400C3—H30.9300O6—H60B0.8400O4—Zn1—O5 ⁱ 110.48 (8)C5—C6—H6119.5O4—Zn1—O1101.48 (8)C1—C6—H6119.5O5 ⁱ —Zn1—O1104.35 (8)O1—C7—N1124.8 (2)O4—Zn1—N2129.69 (9)O1—C7—C1119.0 (2)O5 ⁱ —Zn1—N2117.57 (9)N1—C7—C1116.3 (2)O1—Zn1—N280.84 (8)N2—C8—C9126.0 (2)O4—Zn1—O374.54 (7)N2—C8—H8117.0O5 ⁱ —Zn1—O3104.79 (7)C9—C8—H8117.0O1—Zn1—O3150.04 (8)C14—C9—C10117.5 (3)N2—Zn1—O379.67 (8)C14—C9—C8116.5 (3)C7—O1—Zn1110.12 (16)C10—C9—C8125.9 (2)C2—O2—H20109 (3)O3—C10—C11122.6 (2)C10—O3—C15119.63 (19)O3—C10—C9116.6 (2)C10—O3—C15119.63 (19)O3—C10—C9102.0 (2)	C1—C7		1.476 (4)	C15–	-H15A	0.9	700
C3-C41.365 (6)O6-H60A0.8400C3-H30.9300O6-H60B0.8400O4-Zn1-O5 ⁱ 110.48 (8)C5-C6-H6119.5O4-Zn1-O1101.48 (8)C1-C6-H6119.5O5 ⁱ -Zn1-O1104.35 (8)O1-C7-N1124.8 (2)O4-Zn1-N2129.69 (9)O1-C7-C1119.0 (2)O5 ⁱ -Zn1-N2117.57 (9)N1-C7-C1116.3 (2)O4-Zn1-O374.54 (7)N2-C8-C9126.0 (2)O4-Zn1-O3104.79 (7)C9-C8-H8117.0O5 ⁱ -Zn1-O3150.04 (8)C14-C9-C10117.5 (3)N2-Zn1-O379.67 (8)C14-C9-C8116.5 (3)C7-O1-Zn1110.12 (16)C10-C9-C8125.9 (2)C2-O2-H20109 (3)O3-C10-C11122.6 (2)C10-O3-C15119.63 (19)O3-C10-C9116.6 (2)	C2—C3		1.400 (5)	C15–	-H15B	0.9	700
C3—H30.9300O6—H60B0.8400 $O4$ —Zn1—OS ⁱ 110.48 (8)C5—C6—H6119.5 $O4$ —Zn1—O1101.48 (8)C1—C6—H6119.5 $O5^i$ —Zn1—O1104.35 (8)O1—C7—N1124.8 (2) $O4$ —Zn1—N2129.69 (9)O1—C7—C1119.0 (2) $O5^i$ —Zn1—N2117.57 (9)N1—C7—C1116.3 (2) $O1$ —Zn1—N280.84 (8)N2—C8—C9126.0 (2) $O4$ —Zn1—O374.54 (7)N2—C8—H8117.0 $O5^i$ —Zn1—O3104.79 (7)C9—C8—H8117.0 $O1$ —Zn1—O379.67 (8)C14—C9—C10117.5 (3) $N2$ —Zn1—O379.67 (8)C14—C9—C8116.5 (3) $C7$ —O1—Zn1110.12 (16)C10—C9—C8125.9 (2) $C2$ —O2—H20109 (3)O3—C10—C11122.6 (2) $C10$ —O3—C15119.63 (19)O3—C10—C9116.6 (2) $C10$ — $O3$ —Zn1127.81 (15)C14—C10—C9116.6 (2)	C3—C4		1.365 (6)	06—	H60A	0.84	400
$O4-Zn1-O5^i$ 110.48 (8) $C5-C6-H6$ 119.5 $O4-Zn1-O1$ 101.48 (8) $C1-C6-H6$ 119.5 $O5^i-Zn1-O1$ 104.35 (8) $O1-C7-N1$ 124.8 (2) $O4-Zn1-N2$ 129.69 (9) $O1-C7-C1$ 119.0 (2) $O5^i-Zn1-N2$ 117.57 (9) $N1-C7-C1$ 116.3 (2) $O1-Zn1-N2$ 80.84 (8) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O1-Zn1-O3$ 79.67 (8) $C14-C9-C10$ 117.5 (3) $N2-Zn1-O3$ 79.67 (8) $C14-C9-C8$ 125.9 (2) $C2-O2-H20$ 109 (3) $O3-C10-C11$ 122.6 (2) $C10-O3-C15$ 119.63 (19) $O3-C10-C9$ 126.0 (2)	С3—Н3		0.9300	O6—	H60B	0.84	400
$O4-Zn1-O1$ $101.48 (8)$ $C1-C6-H6$ 119.5 $O5^i-Zn1-O1$ $104.35 (8)$ $O1-C7-N1$ $124.8 (2)$ $O4-Zn1-N2$ $129.69 (9)$ $O1-C7-C1$ $119.0 (2)$ $O5^i-Zn1-N2$ $117.57 (9)$ $N1-C7-C1$ $116.3 (2)$ $O1-Zn1-N2$ $80.84 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $74.54 (7)$ $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $150.04 (8)$ $C14-C9-C10$ $117.5 (3)$ $N2-Zn1-O3$ $79.67 (8)$ $C14-C9-C8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 (3)$ $O3-C10-C11$ $122.6 (2)$ $C10-O3-C15$ $119.63 (19)$ $O3-C10-C9$ $116.6 (2)$	04—Zn1—03	5 ⁱ	110.48 (8)	С5—	С6—Н6	119	.5
$O5^{i}$ —Zn1—O1104.35 (8)O1—C7—N1124.8 (2) $O4$ —Zn1—N2129.69 (9)O1—C7—C1119.0 (2) $O5^{i}$ —Zn1—N2117.57 (9)N1—C7—C1116.3 (2) $O1$ —Zn1—N280.84 (8)N2—C8—C9126.0 (2) $O4$ —Zn1—O374.54 (7)N2—C8—H8117.0 $O5^{i}$ —Zn1—O3104.79 (7)C9—C8—H8117.0 $O1$ —Zn1—O3150.04 (8)C14—C9—C10117.5 (3) $N2$ —Zn1—O379.67 (8)C14—C9—C8116.5 (3) $C7$ —O1—Zn1110.12 (16)C10—C9—C8125.9 (2) $C2$ —O2—H20109 (3)O3—C10—C11122.6 (2) $C10$ —O3—C15119.63 (19)O3—C10—C9116.6 (2) $C10$ —O3—Tn1127.81 (15)C11—C10C10—C9	O4—Zn1—O	1	101.48 (8)	C1—	С6—Н6	119	.5
$O4-Zn1-N2$ $129.69 (9)$ $O1-C7-C1$ $119.0 (2)$ $O5^i-Zn1-N2$ $117.57 (9)$ $N1-C7-C1$ $116.3 (2)$ $O1-Zn1-N2$ $80.84 (8)$ $N2-C8-C9$ $126.0 (2)$ $O4-Zn1-O3$ $74.54 (7)$ $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79 (7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $150.04 (8)$ $C14-C9-C10$ $117.5 (3)$ $N2-Zn1-O3$ $79.67 (8)$ $C14-C9-C8$ $116.5 (3)$ $C7-O1-Zn1$ $110.12 (16)$ $C10-C9-C8$ $125.9 (2)$ $C2-O2-H20$ $109 (3)$ $O3-C10-C11$ $122.6 (2)$ $C10-O3-C15$ $119.63 (19)$ $O3-C10-C9$ $116.6 (2)$	O5 ⁱ —Zn1—O	1	104.35 (8)	01—	C7—N1	124	.8 (2)
$O5^{i}$ —Zn1—N2117.57 (9)N1—C7—C1116.3 (2) $O1$ —Zn1—N280.84 (8)N2—C8—C9126.0 (2) $O4$ —Zn1—O374.54 (7)N2—C8—H8117.0 $O5^{i}$ —Zn1—O3104.79 (7)C9—C8—H8117.0 $O1$ —Zn1—O3150.04 (8)C14—C9—C10117.5 (3) $N2$ —Zn1—O379.67 (8)C14—C9—C8116.5 (3) $C7$ —O1—Zn1110.12 (16)C10—C9—C8125.9 (2) $C2$ —O2—H20109 (3)O3—C10—C11122.6 (2) $C10$ —O3—C15119.63 (19)O3—C10—C9116.6 (2) $C10$ —O3—Tn1127.81 (15)C11—C10—C0120.9 (2)	O4—Zn1—N2	2	129.69 (9)	01—	C7—C1	119	.0 (2)
$O1-Zn1-N2$ 80.84 (8) $N2-C8-C9$ 126.0 (2) $O4-Zn1-O3$ 74.54 (7) $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ 104.79 (7) $C9-C8-H8$ 117.0 $O1-Zn1-O3$ 150.04 (8) $C14-C9-C10$ 117.5 (3) $N2-Zn1-O3$ 79.67 (8) $C14-C9-C8$ 116.5 (3) $C7-O1-Zn1$ 110.12 (16) $C10-C9-C8$ 125.9 (2) $C2-O2-H20$ 109 (3) $O3-C10-C11$ 122.6 (2) $C10-O3-C15$ 119.63 (19) $O3-C10-C9$ 116.6 (2) $C10-O3-C15$ 127.81 (15) $C11-C10-C9$ $C10-C9$	O5 ⁱ —Zn1—N	2	117.57 (9)	N1—	C7—C1	116	.3 (2)
$O4-Zn1-O3$ $74.54(7)$ $N2-C8-H8$ 117.0 $O5^i-Zn1-O3$ $104.79(7)$ $C9-C8-H8$ 117.0 $O1-Zn1-O3$ $150.04(8)$ $C14-C9-C10$ $117.5(3)$ $N2-Zn1-O3$ $79.67(8)$ $C14-C9-C8$ $116.5(3)$ $C7-O1-Zn1$ $110.12(16)$ $C10-C9-C8$ $125.9(2)$ $C2-O2-H20$ $109(3)$ $O3-C10-C11$ $122.6(2)$ $C10-O3-C15$ $119.63(19)$ $O3-C10-C9$ $116.6(2)$	O1—Zn1—N2	2	80.84 (8)	N2—	С8—С9	126	.0 (2)
$O5^{i}$ —Zn1—O3 $104.79(7)$ C9—C8—H8 117.0 $O1$ —Zn1—O3 $150.04(8)$ $C14$ —C9—C10 $117.5(3)$ $N2$ —Zn1—O3 $79.67(8)$ $C14$ —C9—C8 $116.5(3)$ $C7$ —O1—Zn1 $110.12(16)$ $C10$ —C9—C8 $125.9(2)$ $C2$ —O2—H20 $109(3)$ $O3$ —C10—C11 $122.6(2)$ $C10$ —O3—C15 $119.63(19)$ $O3$ —C10—C9 $116.6(2)$ $C10$ —O3 $Zn1$ $127.81(15)$ $C11$ —C10 $C0$	04—Zn1—03	3	74.54 (7)	N2—	C8—H8	117	.0
O1-Zn1-O3 150.04 (8) $C14-C9-C10$ 117.5 (3) $N2-Zn1-O3$ 79.67 (8) $C14-C9-C8$ 116.5 (3) $C7-O1-Zn1$ 110.12 (16) $C10-C9-C8$ 125.9 (2) $C2-O2-H20$ 109 (3) $O3-C10-C11$ 122.6 (2) $C10-O3-C15$ 119.63 (19) $O3-C10-C9$ 116.6 (2) $C10-O3-T15$ 127.81 (15) $C11-C10-C9$ 120.9 (2)	$O5^{i}$ —Zn1—O	3	104.79 (7)	С9—	С8—Н8	117	.0
N2—Zn1—O3 $79.67 (8)$ C14—C9—C8116.5 (3)C7—O1—Zn1110.12 (16)C10—C9—C8125.9 (2)C2—O2—H20109 (3)O3—C10—C11122.6 (2)C10—O3—C15119.63 (19)O3—C10—C9116.6 (2)C10_O3_Tn1127.81 (15)C11_C10_C9120.9 (2)	O1-Zn1-O2	3	150.04 (8)	C14-	C9C10	117	.5 (3)
C7-O1-Zn1 110.12 (16) C10-C9-C8 125.9 (2) C2-O2-H20 109 (3) O3-C10-C11 122.6 (2) C10-O3-C15 119.63 (19) O3-C10-C9 116.6 (2) C10-O3-Zn1 127.81 (15) C11 C10-C9	N2—Zn1—O3	3	79.67 (8)	C14-		116	.5 (3)
C2—O2—H20 109 (3) O3—C10—C11 122.6 (2) C10—O3—C15 119.63 (19) O3—C10—C9 116.6 (2) C10—O3—7n1 127.81 (15) C11—C10—C0 120.0 (2)	C7—O1—Zn1	1	110.12 (16)	C10–	-С9-С8	125	.9 (2)
C10-03-C15 119.63 (19) 03-C10-C9 116.6 (2) C10-03-7n1 127 81 (15) C11-C10-C9 120.0 (2)	С2—О2—Н2	0	109 (3)	03—	C10—C11	122	.6 (2)
$C_{10} = 0.3 - 7n1$ 127.81 (15) $C_{11} = C_{10} = C_{10} = 0.000 (2)$	C10—O3—C	15	119.63 (19)	03—	С10—С9	116	.6 (2)
12/.01(13) $11-010-09$ $120.9(3)$	C10—O3—Zr	11	127.81 (15)	C11–	-С10-С9	120	.9 (3)
C15—O3—Zn1 111.85 (14) C12—C11—C10 119.9 (3)	C15—O3—Zr	11	111.85 (14)	C12-	C11C10	119	.9 (3)
C16—O4—Zn1 121.68 (17) C12—C11—H11 120.0	C16—O4—Zr	11	121.68 (17)	C12-	-C11-H11	120	.0
C16—O5—Zn1 ⁱⁱ 119.40 (17) C10—C11—H11 120.0	C16—O5—Zr	n1 ⁱⁱ	119.40 (17)	C10–	C11H11	120	.0
C7—N1—N2 112.6 (2) C11—C12—C13 120.4 (3)	C7—N1—N2		112.6 (2)	C11–	C12C13	120	.4 (3)
C8—N2—N1 116.1 (2) C11—C12—H12 119.8	C8—N2—N1		116.1 (2)	C11–	-C12-H12	119	.8

C8—N2—Zn1	132.25 (18)	C13—C12—H12	119.8
N1—N2—Zn1	111.50 (16)	C14—C13—C12	119.4 (3)
C2—C1—C6	118.9 (3)	C14—C13—H13	120.3
C2—C1—C7	122.5 (3)	С12—С13—Н13	120.3
C6—C1—C7	118.6 (3)	C13—C14—C9	121.9 (3)
O2—C2—C1	123.4 (3)	C13—C14—H14	119.1
O2—C2—C3	117.4 (3)	C9—C14—H14	119.1
C1—C2—C3	119.2 (4)	O3—C15—C16	107.4 (2)
C4—C3—C2	120.7 (4)	O3—C15—H15A	110.2
С4—С3—Н3	119.7	C16—C15—H15A	110.2
С2—С3—Н3	119.7	O3—C15—H15B	110.2
C3—C4—C5	120.6 (3)	C16—C15—H15B	110.2
С3—С4—Н4	119.7	H15A—C15—H15B	108.5
С5—С4—Н4	119.7	O4—C16—O5	123.9 (3)
C4—C5—C6	119.6 (4)	O4—C16—C15	120.1 (2)
С4—С5—Н5	120.2	O5-C16-C15	115.9 (2)
С6—С5—Н5	120.2	H60A—O6—H60B	113.4
C5—C6—C1	121.0 (3)		
O4—Zn1—O1—C7	-126.34 (18)	C7—C1—C6—C5	179.3 (3)
O5 ⁱ —Zn1—O1—C7	118.79 (18)	Zn1—O1—C7—N1	-4.7 (3)
N2—Zn1—O1—C7	2.52 (18)	Zn1—O1—C7—C1	175.39 (18)
O3—Zn1—O1—C7	-47.4 (3)	N2—N1—C7—O1	4.5 (4)
O4—Zn1—O3—C10	172.7 (2)	N2—N1—C7—C1	-175.7 (2)
O5 ⁱ —Zn1—O3—C10	-79.7 (2)	C2—C1—C7—O1	168.5 (3)
O1—Zn1—O3—C10	86.5 (2)	C6—C1—C7—O1	-12.4 (4)
N2—Zn1—O3—C10	36.3 (2)	C2-C1-C7-N1	-11.4 (4)
O4—Zn1—O3—C15	-17.10 (17)	C6—C1—C7—N1	167.7 (3)
05^{i} —Zn1—O3—C15	90.50 (17)	N1—N2—C8—C9	-172.7 (3)
O1—Zn1—O3—C15	-103.3(2)	Zn1—N2—C8—C9	12.9 (5)
N2—Zn1—O3—C15	-153.49 (18)	N2—C8—C9—C14	-170.7(3)
05^{i} 7n1 -04 - C16	-81.2 (2)	N2—C8—C9—C10	14.4 (5)
01 - Zn1 - 04 - C16	168 6 (2)	C15-O3-C10-C11	-15 1 (4)
$N_2 = Zn_1 = O_4 = C_{16}$	81.0 (2)	Zn1—O3—C10—C11	154.5 (2)
O3—Zn1—O4—C16	19.1 (2)	C15—O3—C10—C9	164.0 (2)
C7—N1—N2—C8	-177.3 (2)	Zn1—O3—C10—C9	-26.5(3)
C7—N1—N2—Zn1	-1.6 (3)	C14—C9—C10—O3	-179.6 (3)
O4—Zn1—N2—C8	-88.4 (3)	C8—C9—C10—O3	-4.7 (4)
$O5^{i}$ —Zn1—N2—C8	72.7 (3)	C14—C9—C10—C11	-0.5 (4)
O1—Zn1—N2—C8	174.2 (3)	C8—C9—C10—C11	174.3 (3)
O3—Zn1—N2—C8	-28.7 (3)	O3—C10—C11—C12	179.4 (2)
O4—Zn1—N2—N1	96.90 (19)	C9—C10—C11—C12	0.4 (4)
$O5^{i}$ —Zn1—N2—N1	-101.94 (17)	C10-C11-C12-C13	0.4 (4)
O1—Zn1—N2—N1	-0.47 (17)	C11—C12—C13—C14	-1.0 (5)
O3—Zn1—N2—N1	156.67 (18)	C12—C13—C14—C9	0.8 (5)
C6—C1—C2—O2	-178.0 (3)	C10-C9-C14-C13	-0.1 (5)
C7—C1—C2—O2	1.2 (5)	C8—C9—C14—C13	-175.4 (3)
C6—C1—C2—C3	3.5 (5)	C10—O3—C15—C16	-175.6 (2)

C7—C1—C2—C3	-177.4 (3)	Zn1—O3—C15—C16	13.3 (2)
O2—C2—C3—C4	178.1 (4)	Zn1—O4—C16—O5	162.7 (2)
C1—C2—C3—C4	-3.2 (6)	Zn1—O4—C16—C15	-18.2 (3)
C2—C3—C4—C5	0.9 (6)	Zn1 ⁱⁱ —O5—C16—O4	-10.5 (4)
C3—C4—C5—C6	1.1 (6)	Zn1 ⁱⁱ —O5—C16—C15	170.31 (18)
C4—C5—C6—C1	-0.7 (5)	O3-C15-C16-O4	0.8 (3)
C2—C1—C6—C5	-1.5 (5)	O3—C15—C16—O5	180.0 (2)
C		11/2	

Symmetry codes: (i) -x+1, y+1/2, -z+1/2; (ii) -x+1, y-1/2, -z+1/2.

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
O2—H20…N1	0.75 (4)	1.92 (4)	2.583 (3)	148 (4)
O6—H60A····O1 ⁱⁱⁱ	0.84	2.22	3.056 (4)	179.
C8—H8····O2 ^{iv}	0.93	2.41	3.316 (4)	164.

Symmetry codes: (iii) x, y+1, z; (iv) -x, y+1/2, -z+1/2.

Fig. 1





Fig. 2