Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ_2-acetato-1:2κ^3O,O':O;2:3κ^3O:-O,O'-tetrakis(μ_2-2-hydroxybenzoato)-1:2κ^4O:O';2:3κ^4O:O'-bis(1,10-phenanthroline)-1κ^2N,N';3κ^2N,N'-trizinc(II)

Jin-Hua Cai,[a] Ying-Hua Xu[b] and Seik Weng Ng[c]*

[a]Department of Chemistry and Life Sciences, Hechi University, Yizhou, Guangxi 546300, People's Republic of China, [b]College of Chemistry, Chongqing Normal University, Chongqing 400047, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

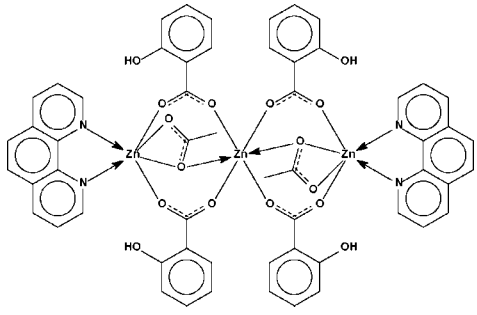
Received 30 October 2007; accepted 31 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.038; wR factor = 0.109; data-to-parameter ratio = 14.9.

The centrosymmetric trinuclear title compound, $[Zn_3(C_2H_3O_2)_2(C_7H_5O_3)_4(C_{12}H_8N_2)_2]$, has six carboxylate groups each bridging two metal centers. The Zn atom on a center of inversion is coordinated by six O atoms in an octahedral environment. The other Zn atoms are each chelated by the *N*-heterocycle, and their coordination number is also six as the acetate group also functions as a chelating group. The hydroxy group of one of the two symmetry-independent salicylate groups is disordered over two positions in a 2:1 ratio.

Related literature

For the structure of the diaquazinc derivative of salicylic acid, see Klug *et al.* (1958). The monomeric 2,2′-bipyridine adduct was reported by Lemoine *et al.* (2004) and the cyclic tetramer by Wang *et al.* (2004)



Experimental

Crystal data

$[Zn_3(C_2H_3O_2)_2(C_7H_5O_3)_4(C_{12}H_8N_2)_2]$
M_r = 1223.05
Monoclinic, $P2_1/n$
a = 10.534 (3) Å
b = 11.682 (3) Å
c = 20.533 (5) Å
β = 91.847 (3)°
V = 2526 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 293 (2) K
0.20 × 0.16 × 0.15 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.524, T_{max} = 0.807
14442 measured reflections
5515 independent reflections
4428 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.109
S = 0.87
5515 reflections
369 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

We are grateful to the Ministry of Education Foundation of the Guangxi Zhuang Autonomous Region for funding this study. We thank Hechi University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2574).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2003). *SMART* (Version 5.625A) and *SAINT* (Version 6.02A). Bruker AXS Inc., Madison, Wisconsin, USA.
Klug, H. P., Alexander, L. E. & Sumner, G. G. (1958). *Acta Cryst.* **11**, 41–46.
Lemoine, P., Bendada, K. & Viossat, B. (2004). *Acta Cryst.* C**60**, m489–m491.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, Y., Odoko, M. & Okabe, N. (2004). *Acta Cryst.* C**60**, m479–m481.
Westrip, S. P. (2007). *publCIF*. In preparation.

  doi:10.1107/S1600536807054852

supplementary materials

Acta Cryst. (2007). E**63**, m2940 [**doi:10.1107/S1600536807054852**]

Di-μ_2-acetato-1:2$\kappa^3O,O':O$;2:3$\kappa^3O:O,O'$-tetrakis(μ_2-2-hydroxybenzoato)-1:2$\kappa^4O:O'$;2:3$\kappa^4O:O'$-bis(1,10-phenanthroline)-1κ^2N,N';3κ^2N,N'-trizinc(II)

J.-H. Cai, Y.-H. Xu and S. W. Ng

Comment

The 2,2'-bipyridine adduct of zinc disalicylate exists in two form, a monomeric form (Lemoine *et al.*, 2004) and a cyclotetrameric form (Wang *et al.*, 2004). The attempt to synthesize the 1,10-phenanthroline analog gave the trinuclear compound in which part of the acetate entity that was present as the counterion is incorporated. The centrosymmetric trinuclear compound has six carboxylate groups each bridging two metal centers. The zinc atom on a center-of-inversion is coordinated to six oxygen atoms in an octahedral environment. The other zinc atoms are each chelated by the *N*-heterocycle, but their coordination number is six as the acetate group that is engaged in bridging also functions as a chelating group (Fig. 1).

Experimental

A solution of salicylic acid (1.0 mmol, 0.138 g) and sodium hydroxde (1.0 mmol, 0.040 g) in methanol (8 ml) was added to a solution of zinc acetate (1.0 mmol, 0.183 g) in methanol (8 ml). 1,10-Phenanthroline (1.0 mmol, 0.180 g), dissolved in methanol (5 ml), was then added. The mixture was placed in a 25-ml Teflon-lined stainless-steel Parr bomb. The bomb was heated at 363 K for five days. Colorless prismatic crystals were collected manually from the cool solution.

Refinement

The hydroxy group of one of the two salicylate groups is disordered over two positions. The phenylene ring was refined as a rigid hexagon of 1.39 Å sides, and the hydroxy group was placed on both *ortho*-positions, subject to the two C–O distances being within 0.01 Å of each other. These were restrained to be nearly coplanar with the ring.

Carbon-hydrogen atoms were placed in calculated positions (C—H 0.93 Å), and were included in the refinement in the riding model approximation, with their temperature factors set to 1.2 times the U_{eq} of the parent atoms.

Figures

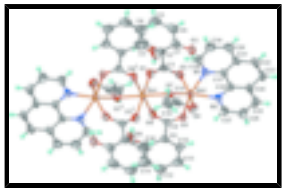


Fig. 1. **Figure 1**. Thermal displacement ellipsoid plot (50% probability) showing the numbering scheme. Hydrogen atoms are drawn as spheres of arbitrary radii; the minor disorder component is not shown.

Di-μ$_2$-acetato-1:2κ^3*O*,*O*':*O*;2:3κ^3*O*:*O*,*O*'-tetrakis(μ$_2$-2- hydroxybenzoato)-1:2κ^4*O*:*O*';2:3κ^4*O*:*O*'-bis(1,10-phenanthroline)- 1κ^2*N*,*N*';3κ^2*N*,*N*'-trizinc(II)

Crystal data

$[Zn_3(C_2H_3O_2)_2(C_7H_5O_3)_4(C_{12}H_8N_2)_2]$	F_{000} = 1248
M_r = 1223.05	D_x = 1.608 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 873 reflections
a = 10.534 (3) Å	θ = 2.6–27.3º
b = 11.682 (3) Å	μ = 1.49 mm^{-1}
c = 20.533 (5) Å	T = 293 (2) K
β = 91.847 (3)º	Prism, colorless
V = 2526 (1) Å^3	0.20 × 0.16 × 0.15 mm
Z = 2	

Data collection

Bruker SMART diffractometer	5515 independent reflections
Radiation source: fine-focus sealed tube	4428 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 295(2) K	θ_{max} = 27.1º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→13
T_{min} = 0.524, T_{max} = 0.807	k = −13→15
14442 measured reflections	l = −22→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.109	$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 2.1051P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.87	$(\Delta/\sigma)_{max}$ = 0.001
5515 reflections	$\Delta\rho_{max}$ = 0.65 e Å^{-3}
369 parameters	$\Delta\rho_{min}$ = −0.66 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.5000	0.5000	0.5000	0.03664 (12)	
Zn2	0.66125 (3)	0.24138 (2)	0.481223 (14)	0.03545 (10)	
O1	0.4523 (2)	0.42396 (19)	0.41149 (10)	0.0558 (5)	
O2	0.52731 (19)	0.24531 (17)	0.40656 (10)	0.0469 (5)	
O3	0.4709 (3)	0.1262 (3)	0.30547 (17)	0.0597 (11)	0.678 (6)
H3O	0.5132	0.1318	0.3395	0.072*	0.678 (6)
O3'	0.3022 (7)	0.4892 (6)	0.3252 (4)	0.129 (6)	0.322 (6)
H3'	0.3424	0.4992	0.3596	0.155*	0.322 (6)
O4	0.4271 (2)	0.36795 (18)	0.55363 (12)	0.0564 (6)	
O5	0.54382 (19)	0.20916 (17)	0.55701 (10)	0.0449 (5)	
O6	0.2546 (3)	0.4024 (2)	0.63370 (17)	0.0939 (11)	
H6O	0.1961	0.4394	0.6486	0.113*	
O7	0.68027 (17)	0.41700 (17)	0.49590 (10)	0.0436 (4)	
O8	0.8313 (2)	0.3264 (2)	0.54866 (12)	0.0654 (6)	
N1	0.8123 (2)	0.23767 (18)	0.41080 (11)	0.0383 (5)	
N2	0.7265 (2)	0.06882 (19)	0.48697 (11)	0.0387 (5)	
C1	0.4616 (2)	0.3288 (2)	0.38461 (13)	0.0402 (6)	
C2	0.3911 (2)	0.3120 (3)	0.32077 (13)	0.0410 (6)	
C3	0.3126 (3)	0.3986 (3)	0.29541 (15)	0.0538 (8)	
H3	0.3066	0.4674	0.3179	0.065*	0.322 (6)
C4	0.2437 (3)	0.3843 (4)	0.23748 (17)	0.0643 (9)	
H4	0.1895	0.4418	0.2222	0.077*	
C5	0.2556 (3)	0.2851 (4)	0.20281 (17)	0.0654 (10)	
H5	0.2105	0.2759	0.1635	0.078*	
C6	0.3336 (4)	0.1993 (4)	0.22567 (17)	0.0666 (10)	
H6	0.3430	0.1331	0.2011	0.080*	
C7	0.3996 (3)	0.2101 (3)	0.28591 (16)	0.0519 (7)	
H7	0.4486	0.1499	0.3024	0.062*	0.678 (6)
C8	0.4555 (3)	0.2705 (2)	0.57659 (13)	0.0382 (6)	
C9	0.3734 (3)	0.2265 (2)	0.62912 (13)	0.0415 (6)	
C10	0.2767 (3)	0.2940 (3)	0.65424 (17)	0.0570 (8)	
C11	0.1974 (4)	0.2487 (4)	0.7010 (2)	0.0700 (10)	
H11	0.1336	0.2936	0.7180	0.084*	
C12	0.2137 (4)	0.1386 (4)	0.72163 (18)	0.0705 (11)	
H12	0.1600	0.1090	0.7525	0.085*	
C13	0.3079 (4)	0.0706 (3)	0.69766 (17)	0.0648 (9)	
H13	0.3177	−0.0046	0.7118	0.078*	
C14	0.3882 (3)	0.1158 (3)	0.65202 (15)	0.0504 (7)	
H14	0.4534	0.0708	0.6365	0.060*	
C15	0.7842 (3)	0.4174 (3)	0.53085 (14)	0.0437 (6)	
C16	0.8460 (3)	0.5300 (3)	0.5450 (2)	0.0737 (11)	
H16A	0.9148	0.5196	0.5762	0.110*	
H16B	0.7849	0.5818	0.5623	0.110*	
H16C	0.8782	0.5612	0.5055	0.110*	
C17	0.8725 (2)	0.1351 (2)	0.40841 (13)	0.0381 (6)	

C18	0.8542 (3)	0.3217 (3)	0.37389 (15)	0.0494 (7)
H18	0.8133	0.3921	0.3750	0.059*
C19	0.9572 (3)	0.3090 (3)	0.33339 (16)	0.0584 (8)
H19	0.9847	0.3705	0.3088	0.070*
C20	1.0167 (3)	0.2069 (3)	0.33018 (17)	0.0587 (8)
H20	1.0847	0.1974	0.3029	0.070*
C21	0.9755 (3)	0.1147 (3)	0.36844 (15)	0.0468 (7)
C22	1.0342 (3)	0.0040 (3)	0.36999 (18)	0.0603 (9)
H22	1.1030	−0.0097	0.3438	0.072*
C23	0.9925 (3)	−0.0803 (3)	0.40818 (18)	0.0567 (8)
H23	1.0324	−0.1513	0.4078	0.068*
C24	0.8880 (3)	−0.0626 (2)	0.44929 (15)	0.0466 (7)
C25	0.8397 (3)	−0.1471 (3)	0.49062 (18)	0.0560 (8)
H25	0.8769	−0.2192	0.4925	0.067*
C26	0.7391 (3)	−0.1231 (3)	0.52754 (19)	0.0581 (8)
H26	0.7064	−0.1790	0.5546	0.070*
C27	0.6841 (3)	−0.0141 (3)	0.52503 (16)	0.0492 (7)
H27	0.6153	0.0010	0.5510	0.059*
C28	0.8269 (2)	0.0453 (2)	0.44954 (13)	0.0380 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0366 (2)	0.0344 (2)	0.0390 (2)	0.00356 (17)	0.00383 (17)	−0.00187 (16)
Zn2	0.03094 (17)	0.03523 (17)	0.04044 (18)	0.00558 (11)	0.00519 (12)	−0.00037 (12)
O1	0.0630 (14)	0.0581 (13)	0.0454 (11)	0.0113 (11)	−0.0103 (10)	−0.0113 (10)
O2	0.0380 (10)	0.0533 (12)	0.0489 (11)	0.0051 (9)	−0.0029 (9)	−0.0045 (9)
O3	0.070 (2)	0.0418 (18)	0.066 (2)	0.0129 (15)	−0.0090 (17)	−0.0103 (15)
O3'	0.197 (14)	0.058 (6)	0.126 (10)	0.027 (7)	−0.093 (9)	−0.004 (5)
O4	0.0528 (13)	0.0425 (11)	0.0755 (15)	0.0102 (9)	0.0252 (11)	0.0150 (10)
O5	0.0420 (11)	0.0445 (10)	0.0490 (11)	0.0098 (9)	0.0151 (9)	0.0066 (9)
O6	0.091 (2)	0.0586 (16)	0.136 (3)	0.0258 (15)	0.064 (2)	0.0017 (16)
O7	0.0328 (9)	0.0445 (10)	0.0535 (11)	0.0034 (8)	0.0017 (8)	−0.0069 (9)
O8	0.0687 (16)	0.0620 (15)	0.0647 (15)	0.0163 (12)	−0.0107 (12)	0.0029 (12)
N1	0.0340 (11)	0.0385 (11)	0.0425 (12)	0.0029 (9)	0.0054 (9)	−0.0004 (9)
N2	0.0295 (11)	0.0382 (11)	0.0485 (13)	0.0000 (9)	0.0031 (9)	−0.0008 (10)
C1	0.0317 (13)	0.0522 (16)	0.0368 (13)	−0.0007 (11)	0.0050 (10)	0.0010 (12)
C2	0.0333 (13)	0.0541 (16)	0.0360 (13)	−0.0066 (12)	0.0057 (11)	−0.0014 (12)
C3	0.0505 (18)	0.066 (2)	0.0440 (16)	−0.0023 (15)	−0.0028 (14)	0.0100 (15)
C4	0.0525 (19)	0.091 (3)	0.0493 (18)	−0.0137 (18)	−0.0038 (15)	0.0202 (18)
C5	0.052 (2)	0.099 (3)	0.0448 (17)	−0.023 (2)	0.0001 (15)	0.0067 (18)
C6	0.064 (2)	0.080 (2)	0.056 (2)	−0.021 (2)	0.0080 (17)	−0.0212 (18)
C7	0.0437 (16)	0.0589 (18)	0.0535 (18)	−0.0064 (14)	0.0071 (14)	−0.0056 (14)
C8	0.0337 (13)	0.0402 (14)	0.0409 (14)	0.0000 (11)	0.0046 (11)	−0.0002 (11)
C9	0.0377 (14)	0.0491 (15)	0.0379 (14)	−0.0026 (12)	0.0056 (11)	−0.0011 (11)
C10	0.0523 (19)	0.0594 (19)	0.0605 (19)	0.0004 (15)	0.0206 (15)	−0.0074 (16)
C11	0.057 (2)	0.088 (3)	0.067 (2)	−0.0026 (18)	0.0285 (18)	−0.0063 (19)
C12	0.059 (2)	0.102 (3)	0.051 (2)	−0.019 (2)	0.0160 (16)	0.0064 (19)

C13	0.064 (2)	0.073 (2)	0.058 (2)	−0.0118 (18)	0.0048 (17)	0.0216 (17)
C14	0.0454 (16)	0.0560 (18)	0.0499 (17)	0.0018 (14)	0.0045 (13)	0.0088 (14)
C15	0.0356 (14)	0.0475 (16)	0.0483 (16)	0.0001 (12)	0.0071 (12)	−0.0066 (12)
C16	0.051 (2)	0.066 (2)	0.105 (3)	−0.0151 (17)	0.009 (2)	−0.028 (2)
C17	0.0296 (12)	0.0433 (14)	0.0415 (14)	0.0036 (10)	0.0022 (10)	−0.0070 (11)
C18	0.0488 (17)	0.0483 (16)	0.0514 (17)	0.0019 (13)	0.0065 (13)	0.0045 (13)
C19	0.0503 (18)	0.069 (2)	0.0561 (19)	−0.0085 (16)	0.0112 (15)	0.0123 (16)
C20	0.0429 (17)	0.078 (2)	0.0565 (19)	0.0025 (16)	0.0166 (14)	−0.0009 (17)
C21	0.0332 (14)	0.0600 (18)	0.0475 (16)	0.0049 (12)	0.0073 (12)	−0.0122 (13)
C22	0.0428 (17)	0.070 (2)	0.069 (2)	0.0168 (15)	0.0123 (15)	−0.0173 (17)
C23	0.0453 (17)	0.0496 (17)	0.075 (2)	0.0146 (14)	0.0012 (15)	−0.0216 (16)
C24	0.0371 (14)	0.0393 (14)	0.0628 (18)	0.0056 (11)	−0.0061 (13)	−0.0117 (13)
C25	0.0543 (19)	0.0330 (14)	0.080 (2)	0.0044 (13)	−0.0091 (16)	−0.0025 (14)
C26	0.0549 (19)	0.0410 (16)	0.078 (2)	−0.0074 (14)	0.0013 (17)	0.0116 (15)
C27	0.0370 (15)	0.0475 (16)	0.0635 (19)	−0.0033 (12)	0.0082 (13)	0.0048 (14)
C28	0.0293 (12)	0.0387 (13)	0.0457 (14)	0.0031 (10)	−0.0012 (11)	−0.0063 (11)

Geometric parameters (Å, °)

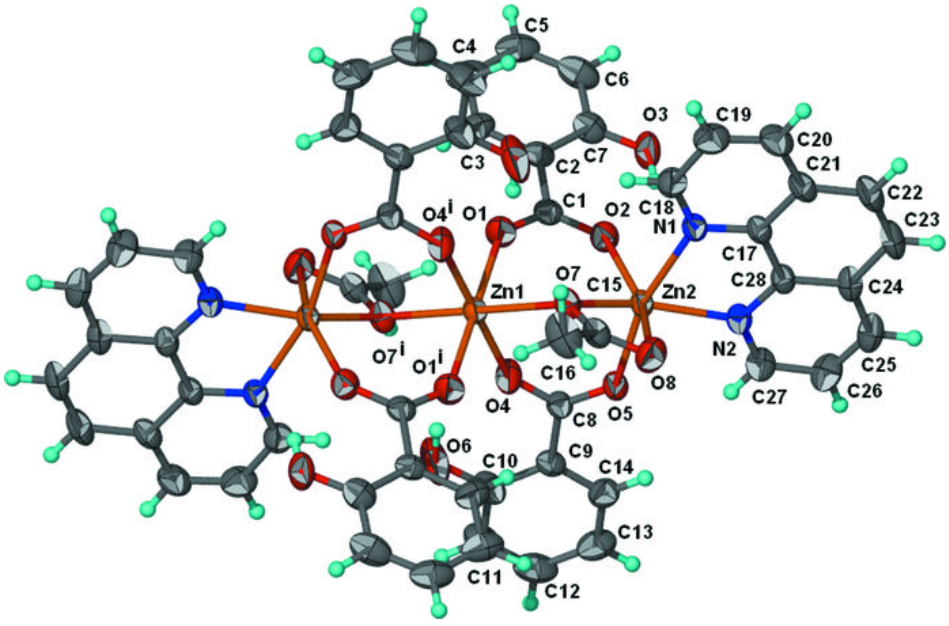
Zn1—O4	2.058 (2)	C6—H6	0.9300
Zn1—O4^{i}	2.058 (2)	C7—H7	0.9300
Zn1—O1^{i}	2.070 (2)	C8—C9	1.496 (4)
Zn1—O1	2.070 (2)	C9—C14	1.382 (4)
Zn1—O7^{i}	2.1362 (19)	C9—C10	1.400 (4)
Zn1—O7	2.1362 (19)	C10—C11	1.396 (5)
Zn2—O2	2.050 (2)	C11—C12	1.363 (6)
Zn2—O5	2.0537 (19)	C11—H11	0.9300
Zn2—O7	2.082 (2)	C12—C13	1.375 (6)
Zn2—N2	2.132 (2)	C12—H12	0.9300
Zn2—N1	2.185 (2)	C13—C14	1.387 (4)
Zn2—O8	2.440 (3)	C13—H13	0.9300
O1—C1	1.246 (3)	C14—H14	0.9300
O2—C1	1.270 (3)	C15—C16	1.492 (4)
O3—C7	1.291 (4)	C16—H16A	0.9600
O3—H3O	0.8200	C16—H16B	0.9600
O3'—C3	1.228 (8)	C16—H16C	0.9600
O3'—H3'	0.8200	C17—C21	1.401 (4)
O4—C8	1.265 (3)	C17—C28	1.439 (4)
O5—C8	1.250 (3)	C18—C19	1.396 (4)
O6—C10	1.353 (4)	C18—H18	0.9300
O6—H6O	0.8200	C19—C20	1.350 (5)
O7—C15	1.290 (3)	C19—H19	0.9300
O8—C15	1.224 (4)	C20—C21	1.410 (5)
N1—C18	1.324 (4)	C20—H20	0.9300
N1—C17	1.357 (3)	C21—C22	1.433 (4)
N2—C27	1.331 (4)	C22—C23	1.342 (5)
N2—C28	1.356 (3)	C22—H22	0.9300
C1—C2	1.499 (4)	C23—C24	1.424 (4)

C2—C7	1.393 (4)	C23—H23	0.9300
C2—C3	1.397 (4)	C24—C25	1.407 (5)
C3—C4	1.384 (5)	C24—C28	1.415 (4)
C3—H3	0.9300	C25—C26	1.352 (5)
C4—C5	1.368 (6)	C25—H25	0.9300
C4—H4	0.9300	C26—C27	1.399 (4)
C5—C6	1.370 (6)	C26—H26	0.9300
C5—H5	0.9300	C27—H27	0.9300
C6—C7	1.405 (5)		
O4—Zn1—O4^{i}	180.00 (8)	C2—C7—C6	119.4 (3)
O4—Zn1—O1^{i}	86.34 (10)	C2—C7—H7	120.3
O4^{i}—Zn1—O1^{i}	93.66 (10)	C6—C7—H7	120.3
O4—Zn1—O1	93.66 (10)	O5—C8—O4	124.4 (3)
O4^{i}—Zn1—O1	86.34 (10)	O5—C8—C9	119.2 (2)
O1^{i}—Zn1—O1	180.0	O4—C8—C9	116.3 (2)
O4—Zn1—O7^{i}	88.39 (8)	C14—C9—C10	118.5 (3)
O4^{i}—Zn1—O7^{i}	91.61 (8)	C14—C9—C8	120.4 (3)
O1^{i}—Zn1—O7^{i}	87.79 (8)	C10—C9—C8	121.1 (3)
O1—Zn1—O7^{i}	92.21 (8)	O6—C10—C11	118.0 (3)
O4—Zn1—O7	91.61 (8)	O6—C10—C9	122.2 (3)
O4^{i}—Zn1—O7	88.39 (8)	C11—C10—C9	119.9 (3)
O1^{i}—Zn1—O7	92.21 (8)	C12—C11—C10	120.0 (4)
O1—Zn1—O7	87.79 (8)	C12—C11—H11	120.0
O7^{i}—Zn1—O7	180.0	C10—C11—H11	120.0
O2—Zn2—O5	98.85 (9)	C11—C12—C13	121.2 (3)
O2—Zn2—O7	98.44 (8)	C11—C12—H12	119.4
O5—Zn2—O7	97.38 (8)	C13—C12—H12	119.4
O2—Zn2—N2	105.98 (8)	C12—C13—C14	119.0 (4)
O5—Zn2—N2	89.18 (8)	C12—C13—H13	120.5
O7—Zn2—N2	153.43 (8)	C14—C13—H13	120.5
O2—Zn2—N1	90.23 (9)	C9—C14—C13	121.4 (3)
O5—Zn2—N1	165.29 (8)	C9—C14—H14	119.3
O7—Zn2—N1	92.67 (8)	C13—C14—H14	119.3
N2—Zn2—N1	77.15 (8)	O8—C15—O7	119.4 (3)
O2—Zn2—O8	152.90 (8)	O8—C15—C16	122.5 (3)
O5—Zn2—O8	95.38 (9)	O7—C15—C16	118.0 (3)
O7—Zn2—O8	56.72 (8)	C15—C16—H16A	109.5
N2—Zn2—O8	97.13 (8)	C15—C16—H16B	109.5
N1—Zn2—O8	81.17 (9)	H16A—C16—H16B	109.5
C1—O1—Zn1	138.7 (2)	C15—C16—H16C	109.5
C1—O2—Zn2	129.52 (18)	H16A—C16—H16C	109.5
C7—O3—H3O	120.0	H16B—C16—H16C	109.5
C3—O3'—H3'	120.0	N1—C17—C21	122.9 (3)
C8—O4—Zn1	141.86 (19)	N1—C17—C28	117.2 (2)
C8—O5—Zn2	127.65 (18)	C21—C17—C28	119.9 (3)
C10—O6—H6O	120.0	N1—C18—C19	122.8 (3)

C15—O7—Zn2	99.21 (17)	N1—C18—H18	118.6
C15—O7—Zn1	135.74 (18)	C19—C18—H18	118.6
Zn2—O7—Zn1	111.80 (9)	C20—C19—C18	119.6 (3)
C15—O8—Zn2	84.32 (18)	C20—C19—H19	120.2
C18—N1—C17	118.0 (2)	C18—C19—H19	120.2
C18—N1—Zn2	128.86 (19)	C19—C20—C21	119.7 (3)
C17—N1—Zn2	113.11 (17)	C19—C20—H20	120.1
C27—N2—C28	117.9 (2)	C21—C20—H20	120.1
C27—N2—Zn2	127.40 (19)	C17—C21—C20	117.0 (3)
C28—N2—Zn2	114.59 (17)	C17—C21—C22	118.8 (3)
O1—C1—O2	125.3 (3)	C20—C21—C22	124.1 (3)
O1—C1—C2	117.4 (3)	C23—C22—C21	121.7 (3)
O2—C1—C2	117.3 (2)	C23—C22—H22	119.1
C7—C2—C3	118.3 (3)	C21—C22—H22	119.1
C7—C2—C1	121.6 (3)	C22—C23—C24	120.9 (3)
C3—C2—C1	120.1 (3)	C22—C23—H23	119.6
O3'—C3—C4	118.6 (6)	C24—C23—H23	119.6
O3'—C3—C2	120.0 (5)	C25—C24—C28	116.7 (3)
C4—C3—C2	121.4 (3)	C25—C24—C23	123.8 (3)
C4—C3—H3	119.3	C28—C24—C23	119.5 (3)
C2—C3—H3	119.3	C26—C25—C24	119.9 (3)
C5—C4—C3	119.7 (4)	C26—C25—H25	120.1
C5—C4—H4	120.2	C24—C25—H25	120.1
C3—C4—H4	120.2	C25—C26—C27	119.9 (3)
C4—C5—C6	120.4 (3)	C25—C26—H26	120.0
C4—C5—H5	119.8	C27—C26—H26	120.0
C6—C5—H5	119.8	N2—C27—C26	122.5 (3)
C5—C6—C7	120.7 (4)	N2—C27—H27	118.7
C5—C6—H6	119.7	C26—C27—H27	118.7
C7—C6—H6	119.7	N2—C28—C24	123.1 (3)
O3—C7—C2	122.4 (3)	N2—C28—C17	117.8 (2)
O3—C7—C6	118.1 (3)	C24—C28—C17	119.1 (2)

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

Fig. 1


C4
C5
C6
O3
C19
C20
C21
C22
C23
C3
C2
C7
C1
O2
C18
N1
C17
C28
C24
O4i
O1
Zn1
O7
C15
Zn2
O7i
O1i
C16
O8
N2
C25
C26
C27
O4
C8
O5
O6
C10
C9
C14
C13
C11
C12