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Poly[aquabis[μ_2-2-(pyridin-4-ylsulfanyl)-acetato]zinc]

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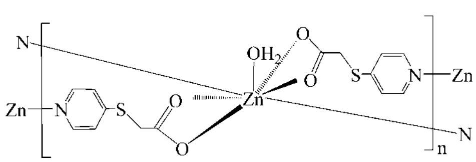
Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.028; *wR* factor = 0.072; data-to-parameter ratio = 12.8.

The crystal structure of the title complex, $[Zn(C_7H_6NO_2S)_2(H_2O)]_n$, consists of extended layers parallel to (001) with 2-(pyridin-4-ylsulfanyl)acetate ligands bridging the Zn^{II} atoms. The Zn^{II} atom shows a distorted pentagonal–bipyramidal coordination environment. The Zn^{II} and one O atom are situated on a crystallographic twofold rotation axis. In the crystal, intralayer O—H···O hydrogen-bond interactions help to consolidate the coordination layer.

Related literature

For metal complexes with polycarboxylate aromatic ligands and their applications, see: Yang *et al.* (2007, 2010); Yu *et al.* (2010). For solid-state structures of metal complexes with pyridine-4-sulfanyl-acetate ligands, see Wang *et al.* (2011); Kondo *et al.* (2002).



Experimental

Crystal data

$[Zn(C_7H_6NO_2S)_2(H_2O)]$
M_r = 419.76
Monoclinic, $C2/c$
a = 16.057 (3) Å
b = 6.3709 (10) Å
c = 15.630 (3) Å
β = 95.393 (4)°
V = 1591.8 (5) Å^3
Z = 4
Mo *K*α radiation
μ = 1.83 mm^{-1}
T = 296 K
0.20 × 0.17 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.711, T_{max} = 0.758
3842 measured reflections
1403 independent reflections
1308 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.04
1403 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3′···O1^{i}	0.82	2.18	2.754 (3)	128

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

Data collection: *APEX2* (Bruker, 2003); 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: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2292).

References

Brandenburg, K. & Berndt, M. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kondo, M., Miyazawa, M., Irie, Y., Shinagawa, R., Horiba, T., Nakamura, A., Naito, T., Maeda, K., Utsuno, S. & Uchida, F. (2002). *Chem. Commun.* pp. 2156–2157.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, J.-Y., Wang, X.-G. & Zhao, X.-J. (2011). *Acta Cryst.* E**67**, m795.
Yang, E.-C., Liu, Z.-Y., Liu, Z.-Y., Zhao, L.-N. & Zhao, X.-J. (2010). *Dalton Trans.* pp. 8868–8871.
Yang, E.-C., Zhao, H.-K., Ding, B., Wang, X.-G. & Zhao, X.-J. (2007). *Cryst. Growth Des.* **7**, 2009–2015.
Yu, Q., Zeng, Y.-F., Zhao, J.-P., Yang, Q., Hu, B.-W., Chang, Z. & Bu, X.-H. (2010). *Inorg. Chem.* **49**, 4301–4306.

supplementary materials

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Poly[aquabis[μ_2-2-(pyridin-4-ylsulfanyl)acetato]zinc]

Z.-C. Wang, B. Ding, X.-G. Wang and X.-J. Zhao

Comment

Recently, metal complexes constructed from aromatic polycarboxylate ligands and transition metal ions have received more and more interest due to their interesting architectures, amazing topologies and potentially technological applications in magnetism (Yang *et al.* 2010), luminesence (Yang *et al.* 2007) and gas storage (Yu *et al.* 2010). The anionic pyridine-4-sulfanyl-acetate ligand has three different potential binding sites upon coordination with metal ions and has exhibited various binding modes through the pyridyl N atom or carboxylate O donors. As a result, diverse complexes with discrete mononuclear (Wang *et al.* 2011), polymeric one-dimensional chains or two-dimensional layers (Kondo *et al.* 2002) have been obtained up to date. As a continuation of this research the crystal structure of a Zn^{II} complex with pyridine-4-sulfanyl-acetate ligands, (I), is reported herein.

A cut-out of the polymeric structure of the title compound showing one Zn^{II} atom in it's complete coordination environment is shown in Fig. 1. The Zn^{II} atom exhibits a distorted pentagonal bipyramidal coordination environment involving two pyridyl N atoms from two separate pyridine-4-sulfanyl-acetate ligands in *trans*-position, four O atoms from a pair of chelating carboxylate groups of pyridine-4-sulfanyl-acetate ligands and one O atom of a terminal water molecule. Each anionic pyridine-4-sulfanyl-acetate ligand acts as a ditopic connector to bridge adjacent Zn^{II} ions by a pyridyl N donor and a bidentate chelating carboxylate to generate a two-dimensional (4, 4) coordination layer with a Zn··· Zn distance of 6.3709 (10) Å. Additionally, O—H ···O hydrogen bonds between the coordinated water molecule and the deprotonated carboxylate (Table 1) help to consolidate the two-dimensional covalent layer (Fig. 2).

Experimental

A methanolic solution of pyridine-4-sulfanyl-acetic acid (50.6 mg, 0.2 mmol) was carefully layered onto a buffer layer of ethyl acetate (2.0 ml) in a straight glass tube below which an aqueous solution containing $Zn(NO_3)_2.6\ H_2O$ (44.6 mg, 0.15 mmol) was placed. The test tube was left in air at room temperature. Colorless block-shaped crystals were harvested within three weeks. Yield: 40% based on Zn^{II} salt. Anal. Calcd. for $C_{14}H_{14}ZnN_2O_5S_2$: C, 40.06; H, 3.36; N, 6.67%. Found: C, 40.12; H, 3.26; N, 6.73%.

Refinement

H atoms could be located from difference Fourier maps, but were subsequently placed in calculated positions and treated as riding, with C–H = 0.93 (aromatic), 0.97 (methylene) and O–H = 0.82 Å. All H atoms were allocated displacement parameters related to those of their parent atoms [U_{iso}(H) = 1.2 U_{eq}(C, O)].

Figures

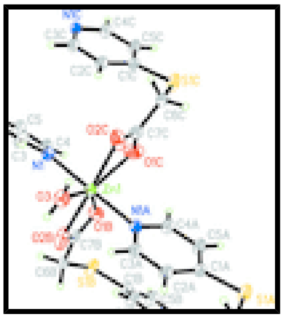


Fig. 1. A portion of the two-dimensional structure of the title comlex. Displacement ellipsoids are drawn at the 30% probablity level. [Symmetry code: (A) 1 – *x*, *y*, 0.5 – *z*; (B) 1/2 + *x*, *y*, 0.5 – *z*; (C) 1/2 - *x*, 1/2 + *y*, 0.5 – *z*]

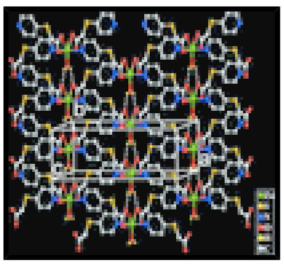


Fig. 2. Part of the two-dimensional chain of (I), with hydrogen bonds shown as dashed lines.

Poly[aquabis[μ_2-2-(pyridin-4-ylsulfanyl)acetato]zinc]

Crystal data

$[Zn(C_7H_6NO_2S)_2(H_2O)]$	$F(000) = 856$
$M_r = 419.76$	$D_x = 1.752$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3018 reflections
a = 16.057 (3) Å	θ = 2.6–27.8°
b = 6.3709 (10) Å	μ = 1.83 mm^{-1}
c = 15.630 (3) Å	*T* = 296 K
β = 95.393 (4)°	Block, colourless
V = 1591.8 (5) Å^3	0.20 × 0.17 × 0.16 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	1403 independent reflections
Radiation source: fine-focus sealed tube	1308 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.016$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -18\rightarrow8$
$T_{min} = 0.711$, $T_{max} = 0.758$	$k = -7\rightarrow7$
3842 measured reflections	$l = -17\rightarrow18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.072$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 2.8608P]$ where $P = (F_o^2 + 2F_c^2)/3$
1403 reflections	$(\Delta/\sigma)_{max} < 0.001$
110 parameters	$\Delta\rho_{max} = 0.57$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.34$ 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}
Zn1	0.5000	0.96825 (6)	0.2500	0.03315 (15)
S1	0.12091 (5)	0.98792 (11)	0.03086 (5)	0.0547 (2)
N1	0.37305 (12)	0.9762 (3)	0.19086 (13)	0.0350 (4)
O1	0.03140 (13)	0.7681 (4)	0.16602 (14)	0.0766 (7)
O2	0.05159 (15)	0.4525 (4)	0.12413 (14)	0.0710 (7)
O3	0.5000	0.6356 (4)	0.2500	0.0511 (7)
H3'	0.4845	0.5927	0.2954	0.077*
C1	0.21478 (15)	0.9755 (4)	0.09745 (16)	0.0366 (5)
C2	0.24687 (15)	0.7966 (4)	0.13868 (17)	0.0429 (6)
H2	0.2162	0.6726	0.1360	0.051*
C3	0.32493 (15)	0.8043 (4)	0.18384 (17)	0.0445 (6)
H3	0.3454	0.6825	0.2111	0.053*
C4	0.34017 (16)	1.1504 (4)	0.15408 (17)	0.0432 (6)
H4	0.3713	1.2735	0.1597	0.052*
C5	0.26277 (16)	1.1574 (4)	0.10832 (18)	0.0458 (6)
H5	0.2425	1.2835	0.0846	0.055*
C6	0.08449 (15)	0.7230 (4)	0.02936 (15)	0.0384 (5)
H6A	0.0389	0.7099	−0.0156	0.046*

H6B	0.1294	0.6325	0.0142	0.046*
C7	0.05446 (15)	0.6435 (5)	0.11276 (16)	0.0481 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0299 (2)	0.0337 (2)	0.0348 (2)	0.000	−0.00208 (15)	0.000
S1	0.0409 (4)	0.0454 (4)	0.0725 (5)	−0.0058 (3)	−0.0227 (3)	0.0140 (3)
N1	0.0325 (10)	0.0370 (11)	0.0346 (10)	−0.0009 (8)	−0.0018 (8)	0.0017 (8)
O1	0.0574 (13)	0.121 (2)	0.0539 (12)	−0.0035 (13)	0.0178 (10)	−0.0277 (13)
O2	0.0762 (16)	0.0738 (16)	0.0580 (13)	−0.0330 (13)	−0.0205 (11)	0.0193 (11)
O3	0.0532 (16)	0.0350 (13)	0.0644 (17)	0.000	0.0022 (13)	0.000
C1	0.0305 (12)	0.0402 (13)	0.0383 (12)	−0.0005 (10)	−0.0013 (10)	0.0013 (10)
C2	0.0331 (13)	0.0370 (14)	0.0574 (15)	−0.0068 (10)	−0.0020 (11)	0.0082 (12)
C3	0.0362 (13)	0.0403 (14)	0.0554 (15)	−0.0010 (11)	−0.0040 (11)	0.0138 (12)
C4	0.0401 (13)	0.0344 (13)	0.0529 (15)	−0.0055 (11)	−0.0067 (11)	0.0005 (11)
C5	0.0428 (14)	0.0321 (13)	0.0598 (16)	0.0004 (11)	−0.0101 (12)	0.0059 (12)
C6	0.0336 (12)	0.0466 (14)	0.0341 (12)	−0.0047 (11)	−0.0023 (9)	−0.0056 (10)
C7	0.0284 (12)	0.077 (2)	0.0368 (13)	−0.0153 (13)	−0.0071 (10)	−0.0071 (14)

Geometric parameters (Å, °)

Zn1—O3	2.119 (3)	O2—Zn1^{iv}	2.208 (3)
Zn1—N1	2.158 (2)	O3—H3'	0.8200
Zn1—N1^{i}	2.158 (2)	C1—C2	1.384 (3)
Zn1—O2^{ii}	2.208 (3)	C1—C5	1.393 (3)
Zn1—O2^{iii}	2.208 (3)	C2—C3	1.380 (3)
Zn1—O1^{ii}	2.398 (3)	C2—H2	0.9300
Zn1—O1^{iii}	2.398 (3)	C3—H3	0.9300
S1—C1	1.751 (2)	C4—C5	1.375 (4)
S1—C6	1.786 (3)	C4—H4	0.9300
N1—C4	1.336 (3)	C5—H5	0.9300
N1—C3	1.338 (3)	C6—C7	1.519 (4)
O1—C7	1.232 (4)	C6—H6A	0.9700
O1—Zn1^{iv}	2.398 (3)	C6—H6B	0.9700
O2—C7	1.231 (4)		
O3—Zn1—N1	91.34 (5)	C7—O2—Zn1^{iv}	96.1 (2)
O3—Zn1—N1^{i}	91.34 (5)	Zn1—O3—H3'	109.5
N1—Zn1—N1^{i}	177.32 (10)	C2—C1—C5	116.8 (2)
O3—Zn1—O2^{ii}	87.40 (6)	C2—C1—S1	125.16 (19)
N1—Zn1—O2^{ii}	87.95 (8)	C5—C1—S1	118.04 (19)
N1^{i}—Zn1—O2^{ii}	92.17 (8)	C3—C2—C1	119.3 (2)
O3—Zn1—O2^{iii}	87.40 (6)	C3—C2—H2	120.4
N1—Zn1—O2^{iii}	92.17 (8)	C1—C2—H2	120.4
N1^{i}—Zn1—O2^{iii}	87.96 (8)	N1—C3—C2	124.1 (2)

O2^{ii}—Zn1—O2^{iii}	174.79 (13)	N1—C3—H3	118.0
O3—Zn1—O1^{ii}	142.81 (5)	C2—C3—H3	118.0
N1—Zn1—O1^{ii}	88.69 (8)	N1—C4—C5	123.5 (2)
N1^{i}—Zn1—O1^{ii}	89.18 (7)	N1—C4—H4	118.2
O2^{ii}—Zn1—O1^{ii}	55.43 (8)	C5—C4—H4	118.2
O2^{iii}—Zn1—O1^{ii}	129.77 (8)	C4—C5—C1	119.9 (2)
O3—Zn1—O1^{iii}	142.81 (5)	C4—C5—H5	120.0
N1—Zn1—O1^{iii}	89.18 (7)	C1—C5—H5	120.0
N1^{i}—Zn1—O1^{iii}	88.69 (8)	C7—C6—S1	115.73 (18)
O2^{ii}—Zn1—O1^{iii}	129.78 (8)	C7—C6—H6A	108.3
O2^{iii}—Zn1—O1^{iii}	55.43 (8)	S1—C6—H6A	108.3
O1^{ii}—Zn1—O1^{iii}	74.38 (11)	C7—C6—H6B	108.3
C1—S1—C6	103.16 (11)	S1—C6—H6B	108.3
C4—N1—C3	116.3 (2)	H6A—C6—H6B	107.4
C4—N1—Zn1	121.53 (16)	O2—C7—O1	121.4 (3)
C3—N1—Zn1	122.05 (16)	O2—C7—C6	118.2 (3)
C7—O1—Zn1^{iv}	87.0 (2)	O1—C7—C6	120.3 (3)
O3—Zn1—N1—C4	−163.91 (19)	C4—N1—C3—C2	2.8 (4)
N1^{i}—Zn1—N1—C4	16.09 (19)	Zn1—N1—C3—C2	−172.8 (2)
O2^{ii}—Zn1—N1—C4	108.7 (2)	C1—C2—C3—N1	0.0 (4)
O2^{iii}—Zn1—N1—C4	−76.5 (2)	C3—N1—C4—C5	−2.4 (4)
O1^{ii}—Zn1—N1—C4	53.3 (2)	Zn1—N1—C4—C5	173.3 (2)
O1^{iii}—Zn1—N1—C4	−21.1 (2)	N1—C4—C5—C1	−0.9 (4)
O3—Zn1—N1—C3	11.5 (2)	C2—C1—C5—C4	3.7 (4)
N1^{i}—Zn1—N1—C3	−168.5 (2)	S1—C1—C5—C4	−174.5 (2)
O2^{ii}—Zn1—N1—C3	−75.8 (2)	C1—S1—C6—C7	70.1 (2)
O2^{iii}—Zn1—N1—C3	99.0 (2)	Zn1^{iv}—O2—C7—O1	−0.1 (3)
O1^{ii}—Zn1—N1—C3	−131.3 (2)	Zn1^{iv}—O2—C7—C6	−177.97 (17)
O1^{iii}—Zn1—N1—C3	154.3 (2)	Zn1^{iv}—O1—C7—O2	0.1 (3)
C6—S1—C1—C2	−1.8 (3)	Zn1^{iv}—O1—C7—C6	177.9 (2)
C6—S1—C1—C5	176.2 (2)	S1—C6—C7—O2	−159.5 (2)
C5—C1—C2—C3	−3.2 (4)	S1—C6—C7—O1	22.6 (3)
S1—C1—C2—C3	174.8 (2)		

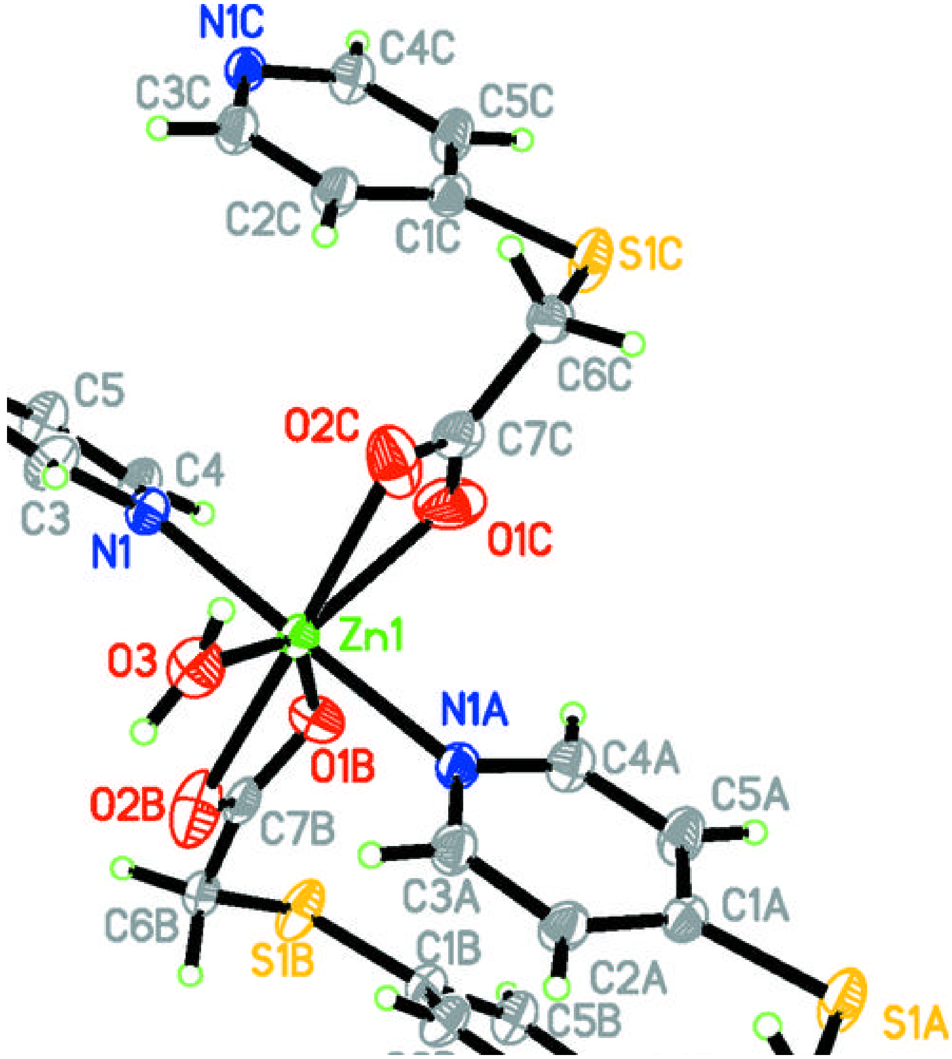
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iii) *x*+1/2, *y*+1/2, *z*; (iv) *x*−1/2, *y*−1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3'···O1^{v}	0.82	2.18	2.754 (3)	128

Symmetry codes: (v) −*x*+1/2, *y*−1/2, −*z*+1/2.

Fig. 1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C3C
C5C
C2C
C1C
S1C
C6C
C5
O2C
C7C
C4
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O1C
Zn1
O3
N1A
C4A
O1B
C5A
O2B
C7B
C3A
C1A
C6B
S1B
C1B
C2A
C5B
S1A

Fig. 2