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ISSN 2414-3146

Hexakis(dimethyl sulfoxide-κO)zinc *mer*-aquatris(dimethyl sulfoxide-κO)(ethanol-κO)-[octadecatungstodiphosphato(V)-κO]zincate(II)–dimethyl sulfoxide–ethanol–water (2/4/2/3)

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Received 5 February 2016
Accepted 10 March 2016

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

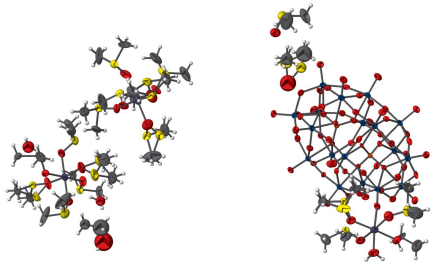
Keywords: crystal structure; Wells–Dawson polyanion; octadecatungstodiphosphate(V); zincate.

CCDC reference: 1463749

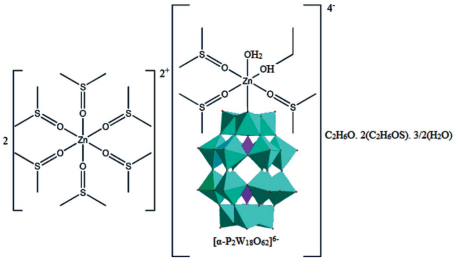
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Zn(C_2H_6OS)_6]_2[Zn(\alpha\text{-}P_2W_{18}O_{62})(C_2H_5OH)(C_2H_6OS)_3(H_2O)]\cdot 2C_2H_6OS\cdot C_2H_5OH\cdot 1.5H_2O$, there are two types of Zn^{II} complex ions. In the $[Zn(\alpha\text{-}P_2W_{18}O_{62})(C_2H_5OH)(C_2H_6OS)_3(H_2O)]^{4-}$ anion, the Zn^{II} cation is coordinated by a Wells–Dawson polyanion $[\alpha\text{-}P_2W_{18}O_{62}]^{6-}$ (POM) *via* a terminal O atom, three dimethyl sulfoxide (DMSO) ligands, one ethanol ligand and one water ligand in a distorted octahedral geometry. The two independent $[Zn(C_2H_6OS)_6]^{2+}$ cations exhibit similar distorted octahedral coordination spheres, and both Zn^{II} cations are coordinated by six DMSO ligands. The crystal packing is governed by extensive O—H···O hydrogen bonds and weak C—H···O hydrogen bonds, forming a three-dimensional supramolecular structure. The S atoms of some DMSO molecules are disordered over two positions with different site-occupancy ratios.

3D view



Chemical scheme



Structure description

The title compound is based on a Wells–Dawson polyanion $(\alpha\text{-}P_2W_{18}O_{62})^{6-}$ (POM) and a zinc coordination complex, and could have catalytic properties (Dolbecq *et al.*, 2010). The molecular structure of the coordination complex cation $[Zn(C_2H_6OS)_6]^{2+}$ is presented in Fig. 1. The Zn1 and Zn3 ions exhibit similar octahedral coordination spheres defined by six O atoms from DMSO ligands. The corresponding Zn—O bond lengths range from 2.054 (8) Å to 2.121 (10) Å.

In the cluster anion $[Zn(\alpha\text{-}P_2W_{18}O_{62})(C_2H_5OH)(C_2H_6OS)_3(H_2O)]^{4-}$ (Fig. 2), the Zn2 ion has also octahedral coordination geometry and is coordinated by the POM *via* a

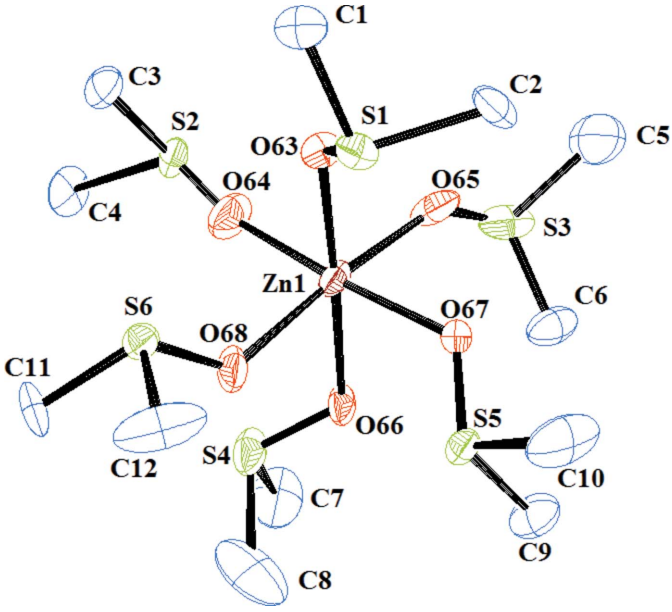


Figure 1
The molecular structure of the Zn1 cationic complex $[Zn(C_2H_6OS)_6]^{2+}$. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

terminal oxygen atom with a Zn2—O9 distance of 2.234 (8) Å, three oxygen atoms from DMSO ligands with Zn2—O bond lengths of 2.061 (10) to 2.070 (10) Å, one O atom from the ethanol ligand [2.114 (9) Å] and one O atom from the water molecule [2.052 (10) Å]; such coordination bond lengths

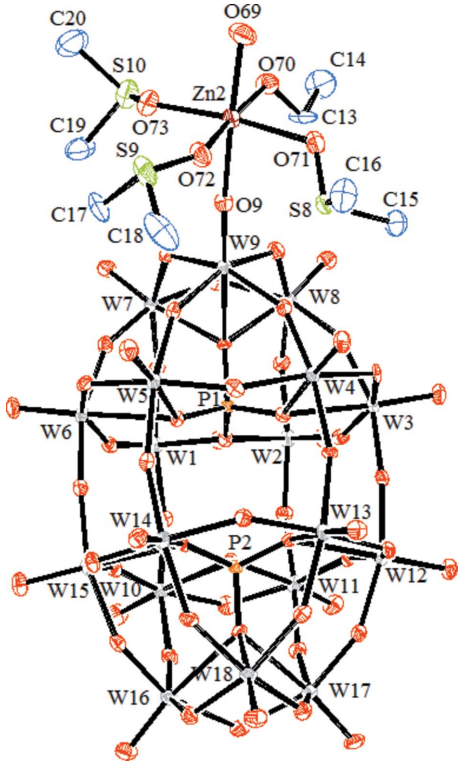


Figure 2
The molecular structure of the anionic complex of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H11W···O79	0.85	2.12	2.934 (19)	162
O1W—H21W···O3^{i}	0.85	2.18	3.005 (19)	165
O2W—H12W···S13	0.85	2.73	3.30 (2)	125
O2W—H12W···O76	0.85	1.87	2.63 (2)	147
O2W—H22W···O17^{ii}	0.85	1.97	2.72 (3)	146
O69—H269···O81^{iii}	0.85	1.96	2.696 (16)	144
O70—HO70···O81^{iii}	0.85	2.18	2.856 (15)	136
C2—H2A···O8^{i}	0.97	2.49	3.313 (19)	143
C2—H2C···O16^{ii}	0.97	2.50	3.330 (19)	144
C3—H3B···O63	0.97	2.57	3.31 (2)	133
C9—H9C···O11^{iv}	0.97	2.55	3.48 (2)	161
C10—H10C···O8^{i}	0.97	2.55	3.36 (2)	141
C11—H11A···O1^{v}	0.97	2.57	3.49 (2)	160
C13—H13A···O32	0.98	2.46	3.345 (16)	150
C15—H15A···O4	0.97	2.36	3.05 (2)	127
C15—H15C···O36^{vi}	0.97	2.57	3.531 (19)	171
C16—H16B···O12^{vi}	0.97	2.58	3.39 (2)	142
C17—H17C···O73	0.97	2.55	3.27 (2)	131
C19—H19A···O33	0.97	2.45	3.36 (2)	158
C23—H23A···O21^{i}	0.97	2.39	3.357 (17)	176
C24—H24A···O32^{i}	0.97	2.57	3.477 (19)	156
C26—H26C···O75	0.97	2.58	3.31 (3)	132
C27—H27A···O34^{iv}	0.97	2.40	3.17 (2)	136
C27—H27B···O17^{ii}	0.97	2.42	3.38 (3)	172
C29—H29A···O7^{vii}	0.97	2.45	3.279 (19)	143
C30—H30B···O74	0.97	2.58	3.192 (18)	121
C30—H30C···O1^{iv}	0.97	2.52	3.449 (16)	159
C31—H31A···O19^{iv}	0.97	2.56	3.195 (17)	123
C32—H32A···O2^{iv}	0.97	2.53	3.365 (18)	144
C33—H33A···O43^{viii}	0.97	2.58	3.50 (2)	159
C37—H37A···S13	0.97	2.80	3.46 (2)	126
C37—H37A···O76	0.97	2.02	2.93 (2)	154

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

values agree with those reported in literature (Tian *et al.*, 2007). The ligands around the Zn2 ion are arranged in a meridional fashion.

The W–O bond lengths, ranging from 1.681 (8) Å to 2.388 (7) Å, agree with those reported for other Wells–Dawson-type polyanions $(\alpha\text{-}P_2W_{18}O_{62})^{6-}$ (Dhifallah *et al.*, 2016).

The complex cation $[Zn(C_2H_6OS)_6]^{2+}$ and cluster anion $[Zn(\alpha\text{-}P_2W_{18}O_{62})(C_2H_5OH)(C_2H_6OS)_3(H_2O)]^{4-}$ are interconnected *via* strong O—H···O and weak C—H···O and C—H···S hydrogen bonds (Table 1) and S···O interactions with distances ranging from 3.15 (1) to 3.16 (1) Å, forming a supramolecular assembly as shown in Fig. 3.

Synthesis and crystallization

The title compound was synthesized at room temperature in DMSO. $Zn(NO_3)_2{\cdot}6H_2O$ salt (0.892 g, 3 mmol) was dissolved in 25 ml of DMSO. Then, potassium polyoxidometalate $K_6(\alpha\text{-}P_2W_{18}O_{62}){\cdot}14H_2O$, synthesized according to Mbomekalle *et al.* (2004) (0.606 g, 0.125 mmol) was added under stirring to the $Zn(NO_3)_2$ solution. The reaction mixture was stirred for half an hour. Single crystals of the title compound, suitable for X-ray crystallographic studies, were obtained within three weeks by diffusion of ethanol through the DMSO solution.

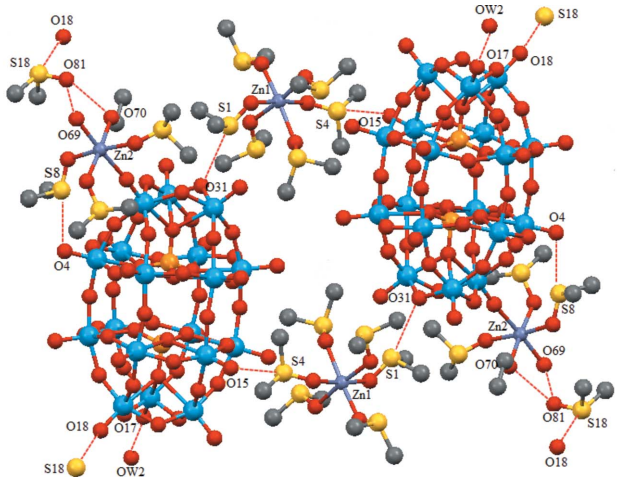


Figure 3
The lattice framework of the title compound, showing supramolecular units assembled *via* hydrogen bonds and O···O and S···O interactions. The Zn3 complex and H atoms have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Restraints and constraints (DELU, SIMU and SADI) in *SHELXL2014* (Sheldrick, 2015) were used in order to maintain a reasonable geometry and atomic displacement parameters for DMSO molecules. The sulfur atoms, (S2, S3, S9, S11 and S14) of five DMSO ligands and the S19 atom of a DMSO solvent molecule, were each disordered over two sites in respective ratios 0.78:0.22; 0.85:0.15; 0.80:0.20; 0.88:0.12; 0.65:0.35 and 0.60:0.40.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_2H_6OS)_6]_2[Zn(P_2W_{18}O_{62})(C_2H_6OS)_3(C_2H_6O)(H_2O)]\cdot 2C_2H_6OS\cdot C_2H_6O\cdot 1.5H_2O$
M_r	6024.70
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, b, c (Å)	17.377 (1), 18.889 (8), 19.705 (6)
α, β, γ (°)	94.766 (2), 90.035 (3), 104.681 (2)
V (Å^3)	6233 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	17.50
Crystal size (mm)	0.20 × 0.18 × 0.03
Data collection	
Diffractometer	Bruker–Nonius KappaCCD
Absorption correction	Multi-scan (*SORTAV*; Blessing, 1995)
T_{min}, T_{max}	0.107, 0.237
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	117368, 27441, 19368
R_{int}	0.097
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.131, 0.98
No. of reflections	27441
No. of parameters	1459
No. of restraints	44
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.22, −3.34

Computer programs: *COLLECT* (Nonius, 2002), *DENZO/SCALEPACK* (Otwinowski & Minor, 1997), *SORTAV* (Blessing, 1995), *CALC-OH* (Nardelli, 1999), *SIR2004* (Burla *et al.*, 2005), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012).

Acknowledgements

The authors gratefully acknowledge financial support from the Ministry of Higher Education and Scientific Research of Tunisia and acknowledge Dr Michel Giorgi, from the University of Aix-Marseille for the data collection.

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full crystallographic data

IUCrData (2016). **1**, x160406 [doi:10.1107/S2414314616004065]

Hexakis(dimethyl sulfoxide-*κO*)zinc *mer*-aquatris(dimethyl sulfoxide-*κO*)(ethanol-*κO*)[octadecatungstodiphosphato(V)-*κO*]zincate(II)–dimethyl sulfoxide–ethanol–water (2/4/2/3)

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Hexakis(dimethyl sulfoxide-*κO*)zinc(II) *mer*-aquatris(dimethyl sulfoxide-*κO*)(ethanol-*κO*)[octadecatungstodiphosphato(V)-*κO*]zincate(II)–dimethyl sulfoxide–ethanol–water (2/4/2/3)

Crystal data

$[Zn(C_2H_6OS)_6]_2[Zn(P_2W_{18}O_{62})(C_2H_6OS)_3(C_2H_6O)(H_2O)]\cdot 2C_2H_6OS\cdot C_2H_6O\cdot 1.5H_2O$
M_r = 6024.70
Triclinic, $P\overline{1}$
a = 17.377 (1) Å
b = 18.889 (8) Å
c = 19.705 (6) Å
α = 94.766 (2)°
β = 90.035 (3)°
γ = 104.681 (2)°
V = 6233 (3) Å^3
Z = 2
$F(000)$ = 5478
D_x = 3.210 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 117368 reflections
θ = 1.0–30.1°
μ = 17.50 mm^{-1}
T = 223 K
Prism, colorless
0.20 × 0.18 × 0.03 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
φ & ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.107, T_{max} = 0.237
117368 measured reflections
27441 independent reflections
19368 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 27.1°, θ_{min} = 2.1°
h = −24→24
k = −26→23
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.131
S = 0.98
27441 reflections
1459 parameters
44 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 3.22 e Å^{-3}
$\Delta\rho_{min}$ = −3.34 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
W1	0.69139 (3)	0.08588 (3)	0.90578 (2)	0.02521 (11)	
W2	0.88176 (3)	0.07796 (3)	0.89459 (2)	0.02635 (11)	
W3	0.97022 (3)	0.05702 (3)	0.72658 (2)	0.02274 (10)	
W4	0.85745 (3)	0.03864 (3)	0.58448 (2)	0.02183 (10)	
W5	0.64813 (3)	0.04649 (3)	0.59669 (2)	0.02263 (11)	
W6	0.56830 (3)	0.06625 (3)	0.74996 (2)	0.02549 (11)	
W7	0.63011 (3)	−0.09439 (3)	0.80395 (2)	0.02659 (11)	
W8	0.82283 (3)	−0.10040 (3)	0.79098 (2)	0.02621 (11)	
W9	0.70830 (3)	−0.11609 (3)	0.64886 (2)	0.02326 (11)	
W10	0.75050 (3)	0.29067 (3)	0.89805 (2)	0.02707 (11)	
W11	0.94086 (3)	0.28280 (3)	0.88869 (2)	0.02789 (12)	
W12	1.03064 (3)	0.26142 (3)	0.72179 (2)	0.02339 (11)	
W13	0.92015 (3)	0.24284 (3)	0.57792 (2)	0.02189 (10)	
W14	0.71155 (3)	0.25120 (3)	0.58862 (2)	0.02378 (11)	
W15	0.62944 (3)	0.27060 (3)	0.74089 (2)	0.02665 (11)	
W16	0.78916 (3)	0.44130 (3)	0.78387 (2)	0.02834 (12)	
W17	0.98177 (3)	0.43618 (3)	0.77634 (3)	0.02951 (12)	
W18	0.87264 (3)	0.41972 (3)	0.63091 (2)	0.02654 (11)	
P1	0.76835 (16)	0.05641 (15)	0.74258 (13)	0.0168 (5)	
P2	0.83276 (16)	0.27245 (16)	0.73596 (13)	0.0182 (6)	
O1	0.6314 (5)	0.0773 (5)	0.9749 (4)	0.035 (2)	
O2	0.9435 (5)	0.0670 (5)	0.9572 (4)	0.036 (2)	
O3	1.0619 (5)	0.0398 (5)	0.7365 (4)	0.033 (2)	
O4	0.8762 (5)	0.0100 (5)	0.5041 (4)	0.0323 (19)	
O5	0.6005 (5)	0.0197 (5)	0.5187 (4)	0.034 (2)	
O6	0.4709 (5)	0.0547 (5)	0.7699 (4)	0.035 (2)	
O7	0.5534 (5)	−0.1530 (5)	0.8412 (4)	0.035 (2)	
O8	0.8681 (5)	−0.1629 (5)	0.8192 (4)	0.035 (2)	
O9	0.6813 (5)	−0.1896 (5)	0.5887 (4)	0.0300 (19)	
O10	0.7016 (6)	0.3184 (5)	0.9660 (4)	0.042 (2)	
O11	1.0139 (5)	0.3073 (5)	0.9502 (4)	0.038 (2)	
O12	1.1309 (5)	0.2769 (5)	0.7313 (4)	0.032 (2)	
O13	0.9516 (5)	0.2486 (5)	0.4969 (4)	0.0298 (19)	
O14	0.6733 (5)	0.2568 (5)	0.5106 (4)	0.0315 (19)	
O15	0.5432 (5)	0.2924 (5)	0.7585 (4)	0.038 (2)	
O16	0.7510 (6)	0.5104 (5)	0.8157 (4)	0.039 (2)	
O17	1.0648 (5)	0.5015 (5)	0.8008 (5)	0.039 (2)	
O18	0.8869 (5)	0.4760 (5)	0.5662 (4)	0.036 (2)	
O19	0.7868 (5)	0.0738 (5)	0.9453 (3)	0.0293 (19)	

O20	0.9483 (5)	0.0866 (4)	0.8173 (4)	0.0286 (18)
O21	0.9510 (4)	0.0290 (4)	0.6320 (4)	0.0230 (17)
O22	0.7564 (5)	0.0580 (4)	0.5749 (3)	0.0252 (18)
O23	0.5586 (4)	0.0404 (4)	0.6543 (4)	0.0248 (17)
O24	0.6211 (5)	0.0951 (4)	0.8351 (4)	0.0275 (18)
O25	0.6639 (5)	−0.0174 (5)	0.8731 (4)	0.0281 (18)
O26	0.8427 (5)	−0.0245 (4)	0.8631 (4)	0.0289 (18)
O27	0.9058 (5)	−0.0390 (4)	0.7451 (4)	0.0254 (17)
O28	0.8003 (4)	−0.0543 (4)	0.6118 (3)	0.0224 (16)
O29	0.6520 (4)	−0.0507 (4)	0.6197 (4)	0.0233 (17)
O30	0.5769 (5)	−0.0311 (4)	0.7637 (4)	0.0268 (18)
O31	0.7166 (5)	−0.1345 (5)	0.8265 (4)	0.0299 (19)
O32	0.7797 (5)	−0.1510 (5)	0.7052 (4)	0.0307 (19)
O33	0.6286 (5)	−0.1461 (4)	0.7153 (4)	0.0272 (18)
O34	0.8556 (5)	0.3082 (5)	0.9372 (4)	0.0308 (19)
O35	0.9972 (4)	0.2543 (4)	0.8125 (4)	0.0265 (18)
O36	1.0207 (4)	0.2614 (4)	0.6258 (4)	0.0236 (17)
O37	0.8085 (5)	0.2258 (4)	0.5670 (4)	0.0270 (18)
O38	0.6298 (5)	0.2737 (5)	0.6446 (4)	0.0298 (19)
O39	0.6710 (5)	0.2650 (5)	0.8302 (4)	0.0317 (19)
O40	0.7833 (5)	0.3836 (5)	0.8588 (4)	0.0309 (19)
O41	0.9626 (5)	0.3767 (5)	0.8502 (4)	0.0294 (18)
O42	1.0248 (4)	0.3611 (4)	0.7330 (4)	0.0268 (18)
O43	0.9209 (5)	0.3451 (5)	0.5970 (4)	0.0281 (18)
O44	0.7732 (5)	0.3501 (4)	0.6055 (4)	0.0268 (18)
O45	0.6976 (5)	0.3712 (5)	0.7497 (4)	0.0291 (18)
O46	0.9004 (5)	0.4820 (5)	0.8058 (4)	0.0311 (19)
O47	0.9648 (5)	0.4637 (5)	0.6860 (4)	0.0309 (19)
O48	0.8136 (5)	0.4680 (5)	0.6924 (4)	0.0307 (19)
O49	0.7834 (4)	0.0902 (4)	0.8162 (4)	0.0232 (17)
O50	0.8436 (4)	0.0733 (4)	0.7017 (3)	0.0203 (16)
O51	0.6990 (4)	0.0774 (4)	0.7097 (3)	0.0189 (15)
O52	0.7421 (4)	−0.0305 (4)	0.7452 (3)	0.0188 (15)
O53	0.8324 (4)	0.2579 (4)	0.8108 (4)	0.0246 (17)
O54	0.8936 (4)	0.2413 (4)	0.6964 (3)	0.0210 (16)
O55	0.7500 (4)	0.2449 (4)	0.7036 (3)	0.0196 (16)
O56	0.8589 (4)	0.3583 (4)	0.7330 (4)	0.0230 (17)
O57	0.7311 (5)	0.1896 (5)	0.9133 (4)	0.0305 (19)
O58	0.9041 (5)	0.1829 (4)	0.9024 (4)	0.0269 (18)
O59	1.0041 (4)	0.1567 (4)	0.7106 (4)	0.0230 (17)
O60	0.9053 (4)	0.1408 (4)	0.5820 (4)	0.0203 (16)
O61	0.6649 (4)	0.1502 (4)	0.5954 (4)	0.0250 (17)
O62	0.5914 (4)	0.1671 (4)	0.7330 (4)	0.0255 (17)
Zn1	0.65797 (9)	0.67216 (10)	0.04108 (7)	0.0407 (4)
O63	0.6236 (5)	0.6574 (5)	−0.0614 (4)	0.038 (2)
S1	0.6604 (2)	0.7138 (2)	−0.10920 (17)	0.0414 (8)
C1	0.5997 (11)	0.6915 (9)	−0.1838 (8)	0.059 (4)
H1A	0.6206	0.7263	−0.2169	0.089*

H1B	0.5992	0.6423	−0.2027	0.089*	
H1C	0.5459	0.6937	−0.1727	0.089*	
C2	0.7428 (10)	0.6827 (9)	−0.1422 (8)	0.056 (4)	
H2A	0.7707	0.7162	−0.1741	0.083*	
H2B	0.7788	0.6810	−0.1050	0.083*	
H2C	0.7238	0.6340	−0.1654	0.083*	
O64	0.5500 (7)	0.5981 (8)	0.0607 (6)	0.074 (4)	
S2	0.4732 (3)	0.6184 (3)	0.0554 (2)	0.0440 (11)	0.78
C3	0.4339 (10)	0.5852 (12)	−0.0299 (8)	0.070 (6)	0.78
H3A	0.3834	0.5972	−0.0361	0.105*	0.78
H3B	0.4712	0.6084	−0.0630	0.105*	0.78
H3C	0.4262	0.5324	−0.0362	0.105*	0.78
C4	0.4039 (9)	0.5538 (11)	0.0999 (9)	0.067 (5)	0.78
H4A	0.3522	0.5644	0.0982	0.100*	0.78
H4B	0.4000	0.5047	0.0790	0.100*	0.78
H4C	0.4217	0.5571	0.1470	0.100*	0.78
S2A	0.4885 (9)	0.5657 (9)	0.0397 (10)	0.043 (4)	0.22
C3A	0.4339 (10)	0.5852 (12)	−0.0299 (8)	0.070 (6)	0.22
H3A1	0.3836	0.5484	−0.0361	0.105*	0.22
H3A2	0.4240	0.6333	−0.0205	0.105*	0.22
H3A3	0.4645	0.5847	−0.0711	0.105*	0.22
C4A	0.4039 (9)	0.5538 (11)	0.0999 (9)	0.067 (5)	0.22
H4A1	0.3554	0.5257	0.0763	0.100*	0.22
H4A2	0.4149	0.5280	0.1378	0.100*	0.22
H4A3	0.3975	0.6017	0.1169	0.100*	0.22
O65	0.7070 (7)	0.5831 (6)	0.0301 (6)	0.064 (3)	
S3	0.7984 (3)	0.5912 (3)	0.0300 (2)	0.0459 (10)	0.85
C5	0.8090 (16)	0.5036 (15)	−0.0007 (15)	0.133 (12)	0.85
H5A	0.8651	0.5046	−0.0022	0.200*	0.85
H5B	0.7823	0.4674	0.0293	0.200*	0.85
H5C	0.7855	0.4908	−0.0462	0.200*	0.85
C6	0.8278 (11)	0.5957 (10)	0.1169 (8)	0.069 (5)	0.85
H6A	0.8847	0.6008	0.1201	0.104*	0.85
H6B	0.8151	0.6377	0.1417	0.104*	0.85
H6C	0.7998	0.5510	0.1364	0.104*	0.85
S3A	0.7617 (17)	0.5482 (18)	0.0632 (14)	0.066 (7)	0.15
C5A	0.8090 (16)	0.5036 (15)	−0.0007 (15)	0.133 (12)	0.15
H5A1	0.8454	0.4803	0.0205	0.200*	0.15
H5A2	0.7691	0.4667	−0.0277	0.200*	0.15
H5A3	0.8383	0.5395	−0.0300	0.200*	0.15
C6A	0.8278 (11)	0.5957 (10)	0.1169 (8)	0.069 (5)	0.15
H6A1	0.8588	0.5645	0.1339	0.104*	0.15
H6A2	0.8627	0.6353	0.0948	0.104*	0.15
H6A3	0.8021	0.6161	0.1546	0.104*	0.15
O66	0.6908 (5)	0.6965 (7)	0.1435 (4)	0.052 (3)	
S4	0.6307 (3)	0.7146 (3)	0.1922 (2)	0.0732 (15)	
C7	0.6542 (14)	0.6839 (16)	0.2707 (9)	0.113 (10)	
H7A	0.6175	0.6938	0.3051	0.169*	

H7B	0.6497	0.6315	0.2648	0.169*
H7C	0.7081	0.7096	0.2850	0.169*
C8	0.6730 (19)	0.8140 (16)	0.2182 (10)	0.139 (12)
H8A	0.6379	0.8312	0.2502	0.208*
H8B	0.7250	0.8211	0.2396	0.208*
H8C	0.6780	0.8416	0.1783	0.208*
O67	0.7689 (5)	0.7395 (5)	0.0179 (5)	0.044 (2)
S5	0.80429 (19)	0.81711 (19)	0.04867 (17)	0.0370 (7)
C9	0.8720 (11)	0.8095 (10)	0.1130 (9)	0.068 (5)
H9A	0.8968	0.8579	0.1348	0.102*
H9B	0.8437	0.7785	0.1466	0.102*
H9C	0.9126	0.7879	0.0929	0.102*
C10	0.8733 (14)	0.8557 (13)	−0.0099 (10)	0.104 (9)
H10A	0.8989	0.9061	0.0062	0.155*
H10B	0.9130	0.8278	−0.0155	0.155*
H10C	0.8466	0.8548	−0.0534	0.155*
O68	0.6181 (6)	0.7732 (7)	0.0536 (5)	0.061 (3)
S6	0.5558 (2)	0.7983 (2)	0.01869 (16)	0.0391 (8)
C11	0.4924 (10)	0.8187 (11)	0.0812 (10)	0.072 (6)
H11A	0.4503	0.8354	0.0603	0.107*
H11B	0.4692	0.7750	0.1041	0.107*
H11C	0.5221	0.8570	0.1140	0.107*
C12	0.6056 (16)	0.8900 (11)	0.0063 (9)	0.105 (9)
H12A	0.5699	0.9128	−0.0167	0.158*
H12B	0.6222	0.9171	0.0502	0.158*
H12C	0.6519	0.8906	−0.0212	0.158*
Zn2	0.65763 (9)	−0.28099 (9)	0.50579 (7)	0.0355 (3)
O69	0.6403 (7)	−0.3704 (6)	0.4356 (5)	0.061 (3)
H169	0.6388	−0.3810	0.3927	0.073*
H269	0.6510	−0.4058	0.4544	0.073*
O70	0.6996 (6)	−0.3454 (5)	0.5727 (5)	0.045 (2)
HO70	0.6982	−0.3901	0.5610	0.054*
C13	0.7641 (10)	−0.3160 (7)	0.6221 (8)	0.050 (4)
H13A	0.7499	−0.2785	0.6535	0.061*
H13B	0.8120	−0.2923	0.5983	0.061*
C14	0.7812 (13)	−0.3732 (12)	0.6610 (10)	0.084 (6)
H14A	0.8245	−0.3513	0.6934	0.126*
H14B	0.7342	−0.3961	0.6854	0.126*
H14C	0.7963	−0.4099	0.6302	0.126*
O71	0.7749 (6)	−0.2423 (6)	0.4786 (5)	0.050 (3)
S8	0.80568 (19)	−0.16053 (19)	0.46897 (15)	0.0328 (7)
C15	0.9092 (9)	−0.1416 (10)	0.4914 (9)	0.060 (5)
H15A	0.9343	−0.0902	0.4868	0.090*
H15B	0.9150	−0.1523	0.5381	0.090*
H15C	0.9343	−0.1720	0.4614	0.090*
C16	0.8172 (11)	−0.1502 (12)	0.3793 (8)	0.069 (5)
H16A	0.8367	−0.0985	0.3723	0.104*
H16B	0.8549	−0.1766	0.3614	0.104*

H16C	0.7661	−0.1698	0.3558	0.104*	
O72	0.6253 (6)	−0.2148 (6)	0.4385 (5)	0.047 (2)	
S9	0.6102 (3)	−0.1395 (3)	0.4591 (2)	0.0404 (10)	0.8
C17	0.5127 (10)	−0.1582 (11)	0.4896 (10)	0.072 (5)	0.8
H17A	0.4994	−0.1123	0.5036	0.108*	0.8
H17B	0.4758	−0.1850	0.4537	0.108*	0.8
H17C	0.5089	−0.1874	0.5282	0.108*	0.8
C18	0.5966 (14)	−0.1039 (12)	0.3807 (9)	0.086 (7)	0.8
H18A	0.5866	−0.0558	0.3895	0.128*	0.8
H18B	0.6441	−0.0999	0.3539	0.128*	0.8
H18C	0.5515	−0.1367	0.3557	0.128*	0.8
S9A	0.5582 (14)	−0.1865 (15)	0.4157 (11)	0.073 (7)	0.2
C17A	0.5127 (10)	−0.1582 (11)	0.4896 (10)	0.072 (5)	0.2
H17D	0.4683	−0.1393	0.4765	0.108*	0.2
H17E	0.4935	−0.1997	0.5163	0.108*	0.2
H17F	0.5512	−0.1199	0.5164	0.108*	0.2
C18A	0.5966 (14)	−0.1039 (12)	0.3807 (9)	0.086 (7)	0.2
H18D	0.5532	−0.0848	0.3656	0.128*	0.2
H18E	0.6290	−0.0689	0.4147	0.128*	0.2
H18F	0.6290	−0.1118	0.3421	0.128*	0.2
O73	0.5433 (6)	−0.3091 (6)	0.5413 (5)	0.055 (3)	
S10	0.5132 (3)	−0.3393 (3)	0.6070 (2)	0.0631 (12)	
C19	0.4691 (12)	−0.2750 (10)	0.6500 (9)	0.078 (6)	
H19A	0.5080	−0.2416	0.6807	0.116*	
H19B	0.4247	−0.3004	0.6759	0.116*	
H19C	0.4502	−0.2474	0.6171	0.116*	
C20	0.4200 (13)	−0.4014 (12)	0.5842 (14)	0.109 (8)	
H20A	0.3962	−0.4237	0.6244	0.163*	
H20B	0.3850	−0.3751	0.5651	0.163*	
H20C	0.4278	−0.4394	0.5507	0.163*	
O74	1.2758 (6)	0.8563 (7)	−0.2887 (5)	0.060 (3)	
Zn3	1.17765 (9)	0.79421 (9)	−0.24076 (7)	0.0329 (3)	
S11	1.3106 (2)	0.8415 (3)	−0.35584 (19)	0.0424 (10)	0.88
C21	1.2614 (11)	0.8798 (10)	−0.4174 (7)	0.057 (4)	0.88
H21A	1.2824	0.8713	−0.4621	0.085*	0.88
H21B	1.2048	0.8567	−0.4178	0.085*	0.88
H21C	1.2703	0.9322	−0.4057	0.085*	0.88
C22	1.4051 (9)	0.9044 (9)	−0.3534 (8)	0.058 (4)	0.88
H22A	1.4316	0.8980	−0.3959	0.086*	0.88
H22B	1.3989	0.9541	−0.3471	0.086*	0.88
H22C	1.4366	0.8956	−0.3159	0.086*	0.88
S11A	1.3010 (17)	0.8936 (18)	−0.3398 (14)	0.038 (6)*	0.12
C21A	1.2614 (11)	0.8798 (10)	−0.4174 (7)	0.057 (4)	0.12
H21D	1.2923	0.9158	−0.4457	0.085*	0.12
H21E	1.2614	0.8308	−0.4366	0.085*	0.12
H21F	1.2072	0.8846	−0.4155	0.085*	0.12
C22A	1.4051 (9)	0.9044 (9)	−0.3534 (8)	0.058 (4)	0.12
H22D	1.4209	0.9327	−0.3922	0.086*	0.12

H22E	1.4351	0.9298	−0.3132	0.086*	0.12
H22F	1.4155	0.8564	−0.3622	0.086*	0.12
O75	1.1042 (6)	0.8077 (5)	−0.3187 (4)	0.039 (2)	
S12	1.0476 (2)	0.8570 (2)	−0.30924 (15)	0.0378 (8)	
C23	1.0648 (9)	0.9092 (8)	−0.3808 (7)	0.047 (4)	
H23A	1.0307	0.9427	−0.3792	0.070*	
H23B	1.1201	0.9369	−0.3803	0.070*	
H23C	1.0531	0.8765	−0.4222	0.070*	
C24	0.9538 (9)	0.7982 (10)	−0.3364 (8)	0.061 (5)	
H24A	0.9134	0.8254	−0.3320	0.091*	
H24B	0.9564	0.7799	−0.3836	0.091*	
H24C	0.9405	0.7571	−0.3083	0.091*	
O76	1.1859 (7)	0.6921 (6)	−0.2890 (5)	0.063 (3)	
S13	1.1462 (3)	0.6292 (3)	−0.3396 (2)	0.0708 (13)	
C25	1.1681 (15)	0.6690 (14)	−0.4103 (16)	0.150 (14)	
H25A	1.1460	0.6344	−0.4488	0.225*	
H25B	1.1458	0.7112	−0.4099	0.225*	
H25C	1.2254	0.6849	−0.4140	0.225*	
C26	1.0401 (14)	0.6267 (13)	−0.3434 (18)	0.141 (13)	
H26A	1.0127	0.5866	−0.3757	0.212*	
H26B	1.0176	0.6194	−0.2987	0.212*	
H26C	1.0337	0.6728	−0.3579	0.212*	
O77	1.0789 (7)	0.7454 (6)	−0.1868 (5)	0.060 (3)	
S14	1.0575 (4)	0.7247 (4)	−0.1161 (3)	0.0597 (17)	0.65
C27	1.1089 (17)	0.6593 (15)	−0.0962 (10)	0.114 (10)	0.65
H27A	1.0958	0.6451	−0.0506	0.171*	0.65
H27B	1.0933	0.6164	−0.1286	0.171*	0.65
H27C	1.1657	0.6805	−0.0985	0.171*	0.65
C28	0.9552 (12)	0.6652 (13)	−0.1254 (11)	0.090 (7)	0.65
H28A	0.9368	0.6493	−0.0813	0.135*	0.65
H28B	0.9203	0.6923	−0.1431	0.135*	0.65
H28C	0.9547	0.6226	−0.1566	0.135*	0.65
S14A	1.0471 (11)	0.6723 (9)	−0.1693 (7)	0.083 (5)	0.35
C27A	1.1089 (17)	0.6593 (15)	−0.0962 (10)	0.114 (10)	0.35
H27D	1.0893	0.6099	−0.0825	0.171*	0.35
H27E	1.1638	0.6666	−0.1098	0.171*	0.35
H27F	1.1057	0.6946	−0.0583	0.171*	0.35
C28A	0.9552 (12)	0.6652 (13)	−0.1254 (11)	0.090 (7)	0.35
H28D	0.9343	0.6151	−0.1138	0.135*	0.35
H28E	0.9646	0.6981	−0.0841	0.135*	0.35
H28F	0.9171	0.6784	−0.1546	0.135*	0.35
O78	1.2548 (6)	0.7824 (6)	−0.1660 (5)	0.051 (3)	
S15	1.3446 (2)	0.8024 (2)	−0.17201 (17)	0.0440 (9)	
C29	1.3785 (9)	0.7723 (11)	−0.0984 (8)	0.060 (5)	
H29A	1.4362	0.7831	−0.0983	0.090*	
H29B	1.3616	0.7973	−0.0584	0.090*	
H29C	1.3566	0.7197	−0.0979	0.090*	
C30	1.3779 (9)	0.8965 (9)	−0.1497 (7)	0.047 (4)	

H30A	1.4353	0.9116	−0.1529	0.071*	
H30B	1.3540	0.9228	−0.1805	0.071*	
H30C	1.3628	0.9076	−0.1034	0.071*	
O79	1.1753 (6)	0.8982 (6)	−0.1923 (4)	0.046 (2)	
S16	1.1464 (2)	0.9070 (2)	−0.11963 (16)	0.0440 (9)	
C31	1.2085 (11)	0.9914 (9)	−0.0893 (8)	0.064 (5)	
H31A	1.1956	1.0032	−0.0425	0.097*	
H31B	1.2635	0.9887	−0.0912	0.097*	
H31C	1.2010	1.0291	−0.1172	0.097*	
C32	1.0571 (10)	0.9328 (12)	−0.1280 (8)	0.071 (6)	
H32A	1.0353	0.9394	−0.0834	0.107*	
H32B	1.0672	0.9785	−0.1496	0.107*	
H32C	1.0194	0.8947	−0.1559	0.107*	
S18	0.1886 (3)	0.4595 (3)	0.5604 (2)	0.0645 (12)	
O81	0.2625 (6)	0.4510 (6)	0.5251 (6)	0.062 (3)	
C33	0.1090 (11)	0.3857 (13)	0.5239 (14)	0.111 (9)	
H33A	0.0594	0.3886	0.5451	0.166*	
H33B	0.1048	0.3896	0.4753	0.166*	
H33C	0.1199	0.3391	0.5315	0.166*	
C34	0.1934 (13)	0.4212 (15)	0.6378 (9)	0.098 (8)	
H34A	0.1473	0.4243	0.6644	0.146*	
H34B	0.1942	0.3701	0.6289	0.146*	
H34C	0.2414	0.4479	0.6629	0.146*	
S19	0.5479 (5)	0.4255 (5)	0.6467 (4)	0.072 (2)*	0.6
C35	0.4957 (14)	0.4578 (13)	0.5965 (11)	0.092 (7)*	0.6
H35A	0.4764	0.4219	0.5581	0.138*	0.6
H35B	0.4509	0.4685	0.6207	0.138*	0.6
H35C	0.5282	0.5025	0.5801	0.138*	0.6
C36	0.576 (2)	0.490 (2)	0.7078 (19)	0.175 (14)*	0.6
H36A	0.6084	0.4750	0.7409	0.263*	0.6
H36B	0.6069	0.5345	0.6891	0.263*	0.6
H36C	0.5296	0.5005	0.7298	0.263*	0.6
S19A	0.5785 (11)	0.4930 (10)	0.6229 (9)	0.105 (5)*	0.4
C35A	0.4957 (14)	0.4578 (13)	0.5965 (11)	0.092 (7)*	0.4
H35D	0.4941	0.4580	0.5473	0.138*	0.4
H35E	0.4797	0.4076	0.6088	0.138*	0.4
H35F	0.4596	0.4850	0.6162	0.138*	0.4
C36A	0.576 (2)	0.490 (2)	0.7078 (19)	0.175 (14)*	0.4
H36D	0.6287	0.5128	0.7273	0.263*	0.4
H36E	0.5389	0.5173	0.7263	0.263*	0.4
H36F	0.5591	0.4398	0.7188	0.263*	0.4
O82	0.6362 (15)	0.4371 (14)	0.5963 (12)	0.172 (9)*	
C37	1.3200 (12)	0.6351 (11)	−0.2506 (10)	0.077 (5)*	
H37A	1.2764	0.6587	−0.2484	0.116*	
H37B	1.3696	0.6714	−0.2389	0.116*	
H37C	1.3226	0.6129	−0.2965	0.116*	
C38	1.308 (3)	0.583 (2)	−0.206 (2)	0.195 (14)*	
H38A	1.2582	0.5449	−0.2173	0.234*	

H38B	1.3055	0.6039	−0.1594	0.234*	
O83	1.373 (2)	0.5531 (19)	−0.2140 (17)	0.246 (13)*	
H83	1.3747	0.5359	−0.2540	0.296*	
O1W	1.2277 (9)	1.0206 (9)	−0.2780 (7)	0.098 (5)*	
H11W	1.2199	0.9810	−0.2585	0.118*	
H21W	1.1839	1.0329	−0.2786	0.118*	
O2W	1.1829 (14)	0.6271 (13)	−0.1757 (11)	0.064 (6)*	0.5
H12W	1.1739	0.6575	−0.2022	0.077*	0.5
H22W	1.1610	0.5841	−0.1935	0.077*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.0258 (2)	0.0329 (3)	0.0178 (2)	0.0087 (2)	0.00618 (18)	0.00357 (19)
W2	0.0249 (2)	0.0372 (3)	0.0176 (2)	0.0086 (2)	−0.00120 (18)	0.00334 (19)
W3	0.0196 (2)	0.0285 (3)	0.0219 (2)	0.00880 (19)	0.00211 (17)	0.00414 (18)
W4	0.0209 (2)	0.0271 (3)	0.0177 (2)	0.00662 (19)	0.00357 (17)	0.00105 (18)
W5	0.0205 (2)	0.0284 (3)	0.0191 (2)	0.0067 (2)	−0.00084 (17)	0.00162 (18)
W6	0.0189 (2)	0.0340 (3)	0.0237 (2)	0.0067 (2)	0.00360 (18)	0.00349 (19)
W7	0.0252 (2)	0.0273 (3)	0.0265 (2)	0.0041 (2)	0.00822 (19)	0.00579 (19)
W8	0.0253 (2)	0.0278 (3)	0.0268 (2)	0.0073 (2)	−0.00053 (19)	0.00806 (19)
W9	0.0249 (2)	0.0231 (3)	0.0212 (2)	0.0051 (2)	0.00221 (18)	0.00168 (18)
W10	0.0297 (3)	0.0318 (3)	0.0205 (2)	0.0101 (2)	0.00649 (18)	−0.00053 (19)
W11	0.0267 (2)	0.0361 (3)	0.0193 (2)	0.0064 (2)	−0.00222 (18)	−0.00202 (19)
W12	0.0182 (2)	0.0292 (3)	0.0225 (2)	0.00569 (19)	0.00093 (17)	0.00229 (18)
W13	0.0206 (2)	0.0273 (3)	0.0183 (2)	0.00679 (19)	0.00361 (17)	0.00256 (18)
W14	0.0213 (2)	0.0300 (3)	0.0216 (2)	0.0084 (2)	0.00067 (17)	0.00539 (19)
W15	0.0214 (2)	0.0334 (3)	0.0273 (2)	0.0111 (2)	0.00521 (18)	0.0021 (2)
W16	0.0309 (3)	0.0251 (3)	0.0305 (2)	0.0104 (2)	0.0071 (2)	0.0003 (2)
W17	0.0265 (3)	0.0247 (3)	0.0353 (3)	0.0040 (2)	−0.0018 (2)	−0.0009 (2)
W18	0.0306 (3)	0.0236 (3)	0.0260 (2)	0.0072 (2)	0.00503 (19)	0.00456 (19)
P1	0.0185 (13)	0.0166 (15)	0.0157 (12)	0.0048 (11)	0.0020 (10)	0.0036 (10)
P2	0.0200 (14)	0.0179 (15)	0.0163 (12)	0.0049 (12)	0.0010 (10)	−0.0011 (11)
O1	0.032 (5)	0.043 (6)	0.029 (4)	0.009 (4)	0.008 (4)	0.004 (4)
O2	0.034 (5)	0.052 (6)	0.021 (4)	0.012 (4)	−0.002 (4)	0.003 (4)
O3	0.020 (4)	0.043 (6)	0.038 (5)	0.012 (4)	−0.001 (3)	0.001 (4)
O4	0.027 (4)	0.042 (6)	0.028 (4)	0.010 (4)	0.006 (3)	0.005 (4)
O5	0.033 (5)	0.042 (6)	0.028 (4)	0.012 (4)	−0.002 (4)	0.002 (4)
O6	0.023 (4)	0.042 (6)	0.044 (5)	0.014 (4)	0.006 (4)	0.006 (4)
O7	0.040 (5)	0.027 (5)	0.039 (5)	0.008 (4)	0.013 (4)	0.010 (4)
O8	0.039 (5)	0.033 (5)	0.034 (5)	0.008 (4)	0.000 (4)	0.009 (4)
O9	0.034 (5)	0.035 (5)	0.021 (4)	0.009 (4)	0.001 (3)	0.002 (3)
O10	0.048 (6)	0.047 (6)	0.031 (5)	0.010 (5)	0.012 (4)	−0.001 (4)
O11	0.042 (5)	0.042 (6)	0.024 (4)	0.001 (4)	−0.003 (4)	−0.008 (4)
O12	0.021 (4)	0.045 (6)	0.027 (4)	0.008 (4)	−0.008 (3)	−0.005 (4)
O13	0.040 (5)	0.031 (5)	0.019 (4)	0.008 (4)	0.007 (3)	0.000 (3)
O14	0.032 (5)	0.031 (5)	0.031 (4)	0.005 (4)	0.000 (4)	0.005 (4)
O15	0.028 (5)	0.054 (6)	0.038 (5)	0.017 (4)	0.010 (4)	0.008 (4)

O16	0.049 (6)	0.030 (5)	0.038 (5)	0.011 (4)	0.008 (4)	0.002 (4)
O17	0.035 (5)	0.023 (5)	0.053 (6)	−0.004 (4)	−0.006 (4)	0.003 (4)
O18	0.046 (5)	0.029 (5)	0.031 (4)	0.007 (4)	0.004 (4)	0.010 (4)
O19	0.039 (5)	0.037 (5)	0.013 (3)	0.011 (4)	0.001 (3)	0.001 (3)
O20	0.030 (4)	0.026 (5)	0.029 (4)	0.004 (4)	−0.010 (3)	0.003 (3)
O21	0.013 (4)	0.037 (5)	0.023 (4)	0.013 (3)	0.009 (3)	0.007 (3)
O22	0.035 (5)	0.029 (5)	0.015 (3)	0.014 (4)	0.000 (3)	0.007 (3)
O23	0.020 (4)	0.020 (4)	0.033 (4)	0.002 (3)	−0.005 (3)	0.007 (3)
O24	0.030 (4)	0.028 (5)	0.027 (4)	0.012 (4)	0.007 (3)	0.002 (3)
O25	0.026 (4)	0.037 (5)	0.019 (4)	0.003 (4)	0.003 (3)	0.006 (3)
O26	0.027 (4)	0.027 (5)	0.032 (4)	0.005 (4)	−0.004 (3)	0.007 (4)
O27	0.029 (4)	0.025 (5)	0.024 (4)	0.008 (4)	0.001 (3)	0.007 (3)
O28	0.022 (4)	0.027 (5)	0.019 (4)	0.008 (3)	−0.002 (3)	−0.003 (3)
O29	0.016 (4)	0.028 (5)	0.025 (4)	0.004 (3)	0.002 (3)	0.004 (3)
O30	0.023 (4)	0.029 (5)	0.028 (4)	0.007 (4)	0.004 (3)	0.006 (3)
O31	0.031 (4)	0.039 (5)	0.019 (4)	0.006 (4)	0.006 (3)	0.014 (4)
O32	0.030 (5)	0.030 (5)	0.036 (4)	0.012 (4)	0.003 (4)	0.006 (4)
O33	0.022 (4)	0.027 (5)	0.031 (4)	0.003 (4)	0.000 (3)	0.004 (3)
O34	0.036 (5)	0.038 (5)	0.019 (4)	0.011 (4)	−0.001 (3)	−0.002 (3)
O35	0.018 (4)	0.031 (5)	0.029 (4)	0.006 (4)	−0.006 (3)	−0.002 (3)
O36	0.020 (4)	0.024 (4)	0.028 (4)	0.007 (3)	0.007 (3)	0.003 (3)
O37	0.028 (4)	0.028 (5)	0.023 (4)	0.006 (4)	0.000 (3)	−0.004 (3)
O38	0.023 (4)	0.037 (5)	0.034 (4)	0.015 (4)	−0.004 (3)	0.005 (4)
O39	0.035 (5)	0.033 (5)	0.031 (4)	0.015 (4)	0.010 (4)	0.004 (4)
O40	0.029 (5)	0.035 (5)	0.030 (4)	0.014 (4)	−0.002 (3)	−0.008 (4)
O41	0.029 (4)	0.029 (5)	0.027 (4)	0.005 (4)	−0.001 (3)	−0.002 (3)
O42	0.022 (4)	0.029 (5)	0.029 (4)	0.005 (4)	0.007 (3)	0.006 (3)
O43	0.025 (4)	0.029 (5)	0.026 (4)	−0.001 (4)	0.002 (3)	0.005 (3)
O44	0.035 (5)	0.020 (4)	0.028 (4)	0.011 (4)	0.006 (3)	0.007 (3)
O45	0.030 (4)	0.029 (5)	0.032 (4)	0.015 (4)	0.005 (3)	−0.001 (4)
O46	0.038 (5)	0.027 (5)	0.023 (4)	0.001 (4)	0.006 (3)	−0.008 (3)
O47	0.029 (4)	0.031 (5)	0.030 (4)	0.004 (4)	0.010 (3)	0.001 (4)
O48	0.029 (4)	0.029 (5)	0.038 (5)	0.012 (4)	0.006 (4)	0.011 (4)
O49	0.027 (4)	0.023 (4)	0.020 (4)	0.005 (3)	0.008 (3)	0.008 (3)
O50	0.024 (4)	0.021 (4)	0.018 (3)	0.008 (3)	−0.001 (3)	0.003 (3)
O51	0.022 (4)	0.025 (4)	0.010 (3)	0.006 (3)	0.008 (3)	0.003 (3)
O52	0.020 (4)	0.017 (4)	0.018 (3)	0.002 (3)	0.001 (3)	0.000 (3)
O53	0.020 (4)	0.028 (5)	0.025 (4)	0.006 (3)	0.003 (3)	−0.004 (3)
O54	0.022 (4)	0.018 (4)	0.021 (4)	0.000 (3)	0.005 (3)	0.002 (3)
O55	0.015 (4)	0.024 (4)	0.023 (4)	0.010 (3)	0.009 (3)	0.006 (3)
O56	0.019 (4)	0.021 (4)	0.026 (4)	0.000 (3)	0.003 (3)	0.002 (3)
O57	0.036 (5)	0.033 (5)	0.021 (4)	0.006 (4)	0.008 (3)	0.001 (3)
O58	0.032 (4)	0.023 (5)	0.025 (4)	0.005 (4)	0.002 (3)	0.000 (3)
O59	0.020 (4)	0.028 (5)	0.025 (4)	0.012 (3)	0.004 (3)	0.009 (3)
O60	0.025 (4)	0.013 (4)	0.024 (4)	0.004 (3)	0.008 (3)	0.006 (3)
O61	0.018 (4)	0.033 (5)	0.025 (4)	0.006 (3)	0.000 (3)	0.004 (3)
O62	0.021 (4)	0.032 (5)	0.025 (4)	0.008 (4)	0.001 (3)	0.000 (3)
Zn1	0.0236 (7)	0.0593 (11)	0.0332 (8)	−0.0004 (7)	−0.0010 (6)	0.0039 (7)

O63	0.041 (5)	0.038 (6)	0.032 (4)	0.001 (4)	0.000 (4)	0.010 (4)
S1	0.051 (2)	0.036 (2)	0.0357 (17)	0.0083 (17)	0.0056 (15)	0.0019 (15)
C1	0.068 (11)	0.052 (11)	0.054 (9)	0.012 (9)	−0.005 (8)	−0.003 (8)
C2	0.065 (11)	0.047 (10)	0.052 (9)	0.013 (8)	0.028 (8)	−0.007 (7)
O64	0.045 (7)	0.096 (10)	0.068 (8)	−0.008 (7)	0.004 (6)	0.005 (7)
S2	0.029 (2)	0.046 (3)	0.055 (3)	0.007 (2)	0.006 (2)	−0.001 (2)
C3	0.048 (10)	0.116 (17)	0.048 (9)	0.031 (11)	−0.014 (8)	−0.012 (10)
C4	0.040 (9)	0.077 (13)	0.074 (11)	−0.009 (9)	0.029 (8)	0.029 (10)
S2A	0.028 (8)	0.019 (8)	0.084 (12)	0.006 (7)	−0.006 (8)	0.004 (8)
C3A	0.048 (10)	0.116 (17)	0.048 (9)	0.031 (11)	−0.014 (8)	−0.012 (10)
C4A	0.040 (9)	0.077 (13)	0.074 (11)	−0.009 (9)	0.029 (8)	0.029 (10)
O65	0.060 (7)	0.051 (7)	0.071 (7)	0.000 (5)	−0.028 (6)	−0.009 (6)
S3	0.039 (2)	0.047 (3)	0.052 (2)	0.011 (2)	−0.006 (2)	0.008 (2)
C5	0.11 (2)	0.14 (3)	0.16 (3)	0.07 (2)	−0.054 (19)	−0.05 (2)
C6	0.068 (12)	0.068 (12)	0.052 (10)	−0.019 (10)	−0.009 (8)	0.006 (9)
S3A	0.077 (17)	0.061 (17)	0.061 (15)	0.017 (12)	0.021 (13)	0.018 (14)
C5A	0.11 (2)	0.14 (3)	0.16 (3)	0.07 (2)	−0.054 (19)	−0.05 (2)
C6A	0.068 (12)	0.068 (12)	0.052 (10)	−0.019 (10)	−0.009 (8)	0.006 (9)
O66	0.029 (5)	0.097 (9)	0.030 (5)	0.022 (5)	0.006 (4)	−0.002 (5)
S4	0.040 (2)	0.139 (5)	0.041 (2)	0.029 (3)	0.0030 (18)	−0.006 (3)
C7	0.103 (18)	0.21 (3)	0.033 (9)	0.049 (19)	0.006 (10)	0.022 (13)
C8	0.22 (3)	0.17 (3)	0.049 (12)	0.09 (3)	0.050 (16)	0.000 (15)
O67	0.029 (5)	0.050 (6)	0.050 (5)	0.008 (4)	0.002 (4)	−0.013 (5)
S5	0.0279 (16)	0.037 (2)	0.0449 (18)	0.0059 (14)	−0.0055 (14)	0.0033 (15)
C9	0.062 (11)	0.075 (13)	0.064 (11)	0.013 (10)	−0.027 (9)	0.002 (9)
C10	0.110 (18)	0.100 (18)	0.060 (12)	−0.053 (14)	0.013 (11)	0.014 (11)
O68	0.037 (6)	0.113 (10)	0.042 (5)	0.038 (6)	−0.007 (5)	−0.011 (6)
S6	0.0342 (18)	0.046 (2)	0.0356 (17)	0.0083 (16)	−0.0012 (14)	0.0004 (15)
C11	0.048 (10)	0.086 (14)	0.094 (13)	0.046 (10)	0.019 (9)	−0.008 (11)
C12	0.16 (2)	0.064 (14)	0.055 (11)	−0.045 (14)	−0.034 (13)	0.028 (10)
Zn2	0.0314 (8)	0.0365 (9)	0.0392 (8)	0.0111 (7)	−0.0007 (6)	−0.0004 (7)
O69	0.081 (8)	0.054 (7)	0.055 (6)	0.036 (7)	−0.012 (6)	−0.013 (5)
O70	0.054 (6)	0.034 (6)	0.050 (6)	0.015 (5)	−0.007 (5)	0.005 (4)
C13	0.072 (11)	0.018 (7)	0.062 (9)	0.015 (7)	−0.041 (8)	−0.010 (6)
C14	0.090 (16)	0.078 (15)	0.088 (14)	0.027 (13)	−0.020 (12)	0.019 (11)
O71	0.038 (6)	0.049 (7)	0.069 (7)	0.020 (5)	0.010 (5)	0.007 (5)
S8	0.0305 (16)	0.038 (2)	0.0315 (15)	0.0131 (14)	0.0020 (13)	−0.0006 (13)
C15	0.040 (9)	0.061 (11)	0.083 (12)	0.022 (8)	−0.015 (8)	0.004 (9)
C16	0.058 (11)	0.103 (16)	0.045 (9)	0.018 (11)	−0.002 (8)	0.003 (9)
O72	0.044 (6)	0.055 (7)	0.049 (5)	0.026 (5)	−0.008 (4)	0.001 (5)
S9	0.040 (2)	0.045 (3)	0.038 (2)	0.018 (2)	−0.0069 (18)	−0.0013 (19)
C17	0.053 (11)	0.073 (13)	0.102 (14)	0.042 (10)	0.020 (10)	0.003 (11)
C18	0.131 (19)	0.101 (16)	0.053 (10)	0.078 (15)	0.014 (11)	0.022 (10)
S9A	0.059 (12)	0.110 (17)	0.063 (12)	0.058 (12)	−0.043 (10)	−0.039 (11)
C17A	0.053 (11)	0.073 (13)	0.102 (14)	0.042 (10)	0.020 (10)	0.003 (11)
C18A	0.131 (19)	0.101 (16)	0.053 (10)	0.078 (15)	0.014 (11)	0.022 (10)
O73	0.041 (6)	0.060 (7)	0.060 (6)	0.005 (5)	0.004 (5)	0.008 (5)
S10	0.045 (2)	0.074 (3)	0.070 (3)	0.011 (2)	0.003 (2)	0.019 (2)

C19	0.083 (14)	0.058 (12)	0.074 (12)	−0.007 (10)	0.027 (10)	−0.016 (10)
C20	0.081 (16)	0.075 (16)	0.15 (2)	−0.016 (13)	0.036 (15)	−0.018 (15)
O74	0.041 (6)	0.092 (9)	0.034 (5)	−0.011 (6)	0.002 (4)	0.021 (5)
Zn3	0.0294 (7)	0.0425 (9)	0.0255 (7)	0.0054 (7)	−0.0015 (6)	0.0066 (6)
S11	0.035 (2)	0.053 (3)	0.0338 (19)	0.0019 (19)	0.0026 (16)	−0.0003 (18)
C21	0.075 (12)	0.073 (12)	0.025 (7)	0.020 (10)	0.002 (7)	0.013 (7)
C22	0.043 (9)	0.057 (11)	0.059 (10)	−0.014 (8)	0.014 (7)	0.009 (8)
C21A	0.075 (12)	0.073 (12)	0.025 (7)	0.020 (10)	0.002 (7)	0.013 (7)
C22A	0.043 (9)	0.057 (11)	0.059 (10)	−0.014 (8)	0.014 (7)	0.009 (8)
O75	0.049 (6)	0.047 (6)	0.027 (4)	0.024 (5)	−0.009 (4)	−0.001 (4)
S12	0.0432 (19)	0.048 (2)	0.0249 (15)	0.0184 (17)	−0.0018 (13)	−0.0018 (14)
C23	0.058 (10)	0.041 (9)	0.050 (8)	0.026 (8)	0.007 (7)	0.011 (7)
C24	0.033 (8)	0.073 (12)	0.062 (10)	−0.010 (8)	0.013 (7)	−0.002 (9)
O76	0.081 (9)	0.056 (7)	0.054 (6)	0.028 (7)	−0.003 (6)	−0.008 (5)
S13	0.099 (4)	0.060 (3)	0.058 (3)	0.029 (3)	−0.007 (3)	0.006 (2)
C25	0.091 (18)	0.12 (2)	0.24 (3)	−0.007 (16)	−0.04 (2)	0.14 (2)
C26	0.073 (16)	0.061 (15)	0.29 (4)	0.001 (13)	−0.05 (2)	0.05 (2)
O77	0.057 (7)	0.068 (8)	0.044 (6)	−0.010 (6)	0.010 (5)	0.013 (5)
S14	0.073 (4)	0.055 (4)	0.040 (3)	−0.005 (3)	0.013 (3)	0.003 (3)
C27	0.16 (3)	0.14 (2)	0.060 (13)	0.08 (2)	0.010 (14)	0.037 (14)
C28	0.061 (13)	0.108 (19)	0.095 (15)	0.008 (12)	0.005 (11)	0.016 (13)
S14A	0.119 (13)	0.064 (10)	0.054 (8)	−0.002 (9)	0.019 (8)	0.015 (7)
C27A	0.16 (3)	0.14 (2)	0.060 (13)	0.08 (2)	0.010 (14)	0.037 (14)
C28A	0.061 (13)	0.108 (19)	0.095 (15)	0.008 (12)	0.005 (11)	0.016 (13)
O78	0.035 (5)	0.080 (8)	0.039 (5)	0.013 (5)	−0.013 (4)	0.019 (5)
S15	0.0348 (18)	0.060 (3)	0.0373 (18)	0.0094 (17)	−0.0021 (14)	0.0118 (16)
C29	0.032 (8)	0.100 (14)	0.054 (9)	0.019 (9)	−0.006 (7)	0.040 (9)
C30	0.045 (9)	0.063 (11)	0.035 (7)	0.017 (8)	0.000 (6)	0.009 (7)
O79	0.057 (6)	0.052 (7)	0.028 (5)	0.013 (5)	0.004 (4)	0.003 (4)
S16	0.061 (2)	0.039 (2)	0.0268 (16)	0.0034 (18)	−0.0081 (15)	0.0031 (14)
C31	0.079 (13)	0.046 (10)	0.058 (10)	−0.002 (9)	0.004 (9)	−0.003 (8)
C32	0.044 (10)	0.128 (18)	0.037 (8)	0.013 (10)	0.002 (7)	0.006 (9)
S18	0.058 (3)	0.064 (3)	0.078 (3)	0.023 (2)	0.029 (2)	0.021 (2)
O81	0.043 (6)	0.061 (8)	0.085 (8)	0.016 (6)	0.029 (6)	0.015 (6)
C33	0.039 (11)	0.12 (2)	0.17 (2)	−0.008 (12)	0.011 (13)	0.071 (19)
C34	0.076 (14)	0.16 (2)	0.059 (12)	0.019 (15)	0.025 (10)	0.033 (13)

Geometric parameters (Å, º)

W1—O1	1.708 (8)	C9—H9C	0.9700
W1—O57	1.898 (9)	C10—H10A	0.9700
W1—O24	1.899 (8)	C10—H10B	0.9700
W1—O19	1.905 (8)	C10—H10C	0.9700
W1—O25	1.941 (8)	O68—S6	1.478 (10)
W1—O49	2.374 (7)	S6—C11	1.737 (15)
W2—O2	1.694 (8)	S6—C12	1.767 (18)
W2—O20	1.906 (8)	C11—H11A	0.9700
W2—O58	1.913 (8)	C11—H11B	0.9700

W2—O19	1.917 (8)	C11—H11C	0.9700
W2—O26	1.930 (8)	C12—H12A	0.9700
W2—O49	2.370 (7)	C12—H12B	0.9700
W3—O3	1.719 (7)	C12—H12C	0.9700
W3—O59	1.878 (8)	Zn2—O69	2.052 (10)
W3—O20	1.896 (8)	Zn2—O73	2.061 (10)
W3—O21	1.901 (7)	Zn2—O72	2.067 (9)
W3—O27	1.938 (8)	Zn2—O71	2.070 (10)
W3—O50	2.355 (7)	Zn2—O70	2.114 (9)
W4—O4	1.689 (8)	O69—H169	0.8500
W4—O22	1.894 (7)	O69—H269	0.8500
W4—O60	1.902 (7)	O70—C13	1.450 (15)
W4—O28	1.906 (8)	O70—HO70	0.8501
W4—O21	1.932 (7)	C13—C14	1.46 (2)
W4—O50	2.378 (7)	C13—H13A	0.9800
W5—O5	1.720 (8)	C13—H13B	0.9800
W5—O22	1.893 (8)	C14—H14A	0.9700
W5—O61	1.908 (8)	C14—H14B	0.9700
W5—O23	1.911 (8)	C14—H14C	0.9700
W5—O29	1.945 (8)	O71—S8	1.530 (11)
W5—O51	2.368 (6)	S8—C15	1.790 (14)
W6—O6	1.702 (8)	S8—C16	1.800 (16)
W6—O24	1.884 (8)	C15—H15A	0.9700
W6—O62	1.903 (8)	C15—H15B	0.9700
W6—O23	1.904 (8)	C15—H15C	0.9700
W6—O30	1.923 (8)	C16—H16A	0.9700
W6—O51	2.371 (7)	C16—H16B	0.9700
W7—O7	1.712 (9)	C16—H16C	0.9700
W7—O25	1.885 (8)	O72—S9A	1.483 (19)
W7—O30	1.905 (7)	O72—S9	1.532 (10)
W7—O31	1.914 (8)	S9—C17	1.758 (17)
W7—O33	1.926 (8)	S9—C18	1.776 (17)
W7—O52	2.372 (7)	C17—H17A	0.9700
W8—O8	1.703 (8)	C17—H17B	0.9700
W8—O27	1.889 (8)	C17—H17C	0.9700
W8—O26	1.899 (8)	C18—H18A	0.9700
W8—O32	1.924 (8)	C18—H18B	0.9700
W8—O31	1.945 (8)	C18—H18C	0.9700
W8—O52	2.379 (7)	S9A—C17A	1.76 (3)
W9—O9	1.717 (8)	S9A—C18A	1.73 (4)
W9—O29	1.882 (7)	C17A—H17D	0.9700
W9—O28	1.910 (8)	C17A—H17E	0.9700
W9—O33	1.919 (8)	C17A—H17F	0.9700
W9—O32	1.934 (8)	C18A—H18D	0.9700
W9—O52	2.360 (7)	C18A—H18E	0.9700
W10—O10	1.703 (8)	C18A—H18F	0.9700
W10—O39	1.865 (8)	O73—S10	1.500 (11)
W10—O57	1.902 (9)	S10—C19	1.756 (18)

W10—O34	1.921 (8)	S10—C20	1.78 (2)
W10—O40	1.931 (9)	C19—H19A	0.9700
W10—O53	2.376 (7)	C19—H19B	0.9700
W11—O11	1.703 (8)	C19—H19C	0.9700
W11—O58	1.875 (8)	C20—H20A	0.9700
W11—O34	1.903 (8)	C20—H20B	0.9700
W11—O35	1.906 (8)	C20—H20C	0.9700
W11—O41	1.935 (8)	O74—S11A	1.29 (3)
W11—O53	2.357 (7)	O74—S11	1.489 (11)
W12—O12	1.700 (8)	O74—Zn3	2.086 (10)
W12—O35	1.885 (8)	Zn3—O78	2.054 (8)
W12—O36	1.899 (7)	Zn3—O75	2.069 (8)
W12—O42	1.906 (8)	Zn3—O77	2.071 (10)
W12—O59	1.908 (8)	Zn3—O76	2.117 (11)
W12—O54	2.361 (7)	Zn3—O79	2.121 (10)
W13—O13	1.692 (7)	S11—C22	1.764 (15)
W13—O60	1.888 (7)	S11—C21	1.783 (14)
W13—O37	1.894 (8)	C21—H21A	0.9700
W13—O36	1.923 (7)	C21—H21B	0.9700
W13—O43	1.933 (8)	C21—H21C	0.9700
W13—O54	2.381 (7)	C22—H22A	0.9700
W14—O14	1.696 (8)	C22—H22B	0.9700
W14—O61	1.891 (8)	C22—H22C	0.9700
W14—O37	1.904 (8)	S11A—C21A	1.65 (3)
W14—O44	1.906 (8)	S11A—C22A	1.79 (3)
W14—O38	1.909 (8)	C21A—H21D	0.9700
W14—O55	2.383 (7)	C21A—H21E	0.9700
W15—O15	1.681 (8)	C21A—H21F	0.9700
W15—O62	1.891 (8)	C22A—H22D	0.9700
W15—O38	1.903 (8)	C22A—H22E	0.9700
W15—O39	1.924 (8)	C22A—H22F	0.9700
W15—O45	1.962 (9)	O75—S12	1.517 (9)
W15—O55	2.371 (6)	S12—C23	1.771 (14)
W16—O16	1.685 (8)	S12—C24	1.777 (15)
W16—O45	1.876 (8)	C23—H23A	0.9700
W16—O40	1.894 (8)	C23—H23B	0.9700
W16—O46	1.924 (8)	C23—H23C	0.9700
W16—O48	1.931 (8)	C24—H24A	0.9700
W16—O56	2.374 (7)	C24—H24B	0.9700
W17—O17	1.684 (9)	C24—H24C	0.9700
W17—O41	1.891 (8)	O76—S13	1.506 (12)
W17—O46	1.903 (8)	S13—C25	1.64 (2)
W17—O42	1.907 (8)	S13—C26	1.83 (2)
W17—O47	1.939 (8)	C25—H25A	0.9700
W17—O56	2.377 (7)	C25—H25B	0.9700
W18—O18	1.706 (8)	C25—H25C	0.9700
W18—O43	1.892 (8)	C26—H26A	0.9700
W18—O47	1.899 (8)	C26—H26B	0.9700

W18—O48	1.909 (8)	C26—H26C	0.9700
W18—O44	1.924 (8)	O77—S14A	1.423 (18)
W18—O56	2.388 (7)	O77—S14	1.499 (11)
P1—O50	1.513 (8)	S14—C27	1.77 (2)
P1—O51	1.520 (7)	S14—C28	1.85 (2)
P1—O49	1.530 (8)	C27—H27A	0.9700
P1—O52	1.594 (8)	C27—H27B	0.9700
P2—O55	1.520 (7)	C27—H27C	0.9700
P2—O54	1.520 (7)	C28—H28A	0.9700
P2—O53	1.522 (8)	C28—H28B	0.9700
P2—O56	1.574 (8)	C28—H28C	0.9700
O9—Zn2	2.234 (8)	S14A—C28A	1.80 (3)
Zn1—O65	2.066 (12)	S14A—C27A	1.86 (3)
Zn1—O66	2.079 (9)	C27A—H27D	0.9700
Zn1—O63	2.082 (8)	C27A—H27E	0.9700
Zn1—O64	2.094 (12)	C27A—H27F	0.9700
Zn1—O67	2.097 (10)	C28A—H28D	0.9700
Zn1—O68	2.186 (11)	C28A—H28E	0.9700
O63—S1	1.501 (9)	C28A—H28F	0.9700
S1—C1	1.767 (15)	O78—S15	1.516 (10)
S1—C2	1.784 (14)	S15—C30	1.744 (16)
C1—H1A	0.9700	S15—C29	1.754 (13)
C1—H1B	0.9700	C29—H29A	0.9700
C1—H1C	0.9700	C29—H29B	0.9700
C2—H2A	0.9700	C29—H29C	0.9700
C2—H2B	0.9700	C30—H30A	0.9700
C2—H2C	0.9700	C30—H30B	0.9700
O64—S2A	1.146 (18)	C30—H30C	0.9700
O64—S2	1.487 (13)	O79—S16	1.528 (9)
S2—C4	1.773 (15)	S16—C31	1.741 (17)
S2—C3	1.813 (15)	S16—C32	1.752 (17)
C3—H3A	0.9700	C31—H31A	0.9700
C3—H3B	0.9700	C31—H31B	0.9700
C3—H3C	0.9700	C31—H31C	0.9700
C4—H4A	0.9700	C32—H32A	0.9700
C4—H4B	0.9700	C32—H32B	0.9700
C4—H4C	0.9700	C32—H32C	0.9700
S2A—C3A	1.78 (2)	S18—O81	1.499 (10)
S2A—C4A	1.87 (2)	S18—C34	1.752 (19)
C3A—H3A1	0.9700	S18—C33	1.80 (2)
C3A—H3A2	0.9700	C33—H33A	0.9700
C3A—H3A3	0.9700	C33—H33B	0.9700
C4A—H4A1	0.9700	C33—H33C	0.9700
C4A—H4A2	0.9700	C34—H34A	0.9700
C4A—H4A3	0.9700	C34—H34B	0.9700
O65—S3A	1.47 (2)	C34—H34C	0.9700
O65—S3	1.556 (12)	S19—C35	1.60 (2)
S3—C5	1.77 (2)	S19—C36	1.63 (4)

S3—C6	1.777 (16)	S19—O82	1.80 (3)
C5—H5A	0.9700	C35—H35A	0.9700
C5—H5B	0.9700	C35—H35B	0.9700
C5—H5C	0.9700	C35—H35C	0.9700
C6—H6A	0.9700	C36—H36A	0.9700
C6—H6B	0.9700	C36—H36B	0.9700
C6—H6C	0.9700	C36—H36C	0.9700
S3A—C6A	1.60 (3)	S19A—C35A	1.50 (3)
S3A—C5A	1.77 (4)	S19A—C36A	1.68 (4)
C5A—H5A1	0.9699	S19A—O82	1.68 (3)
C5A—H5A2	0.9702	C35A—H35D	0.9700
C5A—H5A3	0.9698	C35A—H35E	0.9700
C6A—H6A1	0.9700	C35A—H35F	0.9700
C6A—H6A2	0.9698	C36A—H36D	0.9700
C6A—H6A3	0.9700	C36A—H36E	0.9700
O66—S4	1.502 (9)	C36A—H36F	0.9700
S4—C7	1.778 (18)	C37—C38	1.36 (4)
S4—C8	1.86 (3)	C37—H37A	0.9700
C7—H7A	0.9700	C37—H37B	0.9700
C7—H7B	0.9700	C37—H37C	0.9700
C7—H7C	0.9700	C38—O83	1.39 (4)
C8—H8A	0.9700	C38—H38A	0.9800
C8—H8B	0.9700	C38—H38B	0.9800
C8—H8C	0.9700	O83—H83	0.8300
O67—S5	1.513 (10)	O1W—H11W	0.8500
S5—C10	1.732 (19)	O1W—H21W	0.8500
S5—C9	1.768 (15)	O2W—H12W	0.8501
C9—H9A	0.9700	O2W—H22W	0.8499
C9—H9B	0.9700		

O1—W1—O57	99.1 (4)	H4B—C4—H4C	109.5
O1—W1—O24	102.4 (4)	O64—S2A—C3A	127.8 (16)
O57—W1—O24	88.5 (3)	O64—S2A—C4A	117.3 (16)
O1—W1—O19	100.4 (4)	C3A—S2A—C4A	95.1 (11)
O57—W1—O19	91.5 (4)	S2A—C3A—H3A1	109.5
O24—W1—O19	156.9 (3)	S2A—C3A—H3A2	109.5
O1—W1—O25	96.7 (4)	H3A1—C3A—H3A2	109.5
O57—W1—O25	163.9 (3)	S2A—C3A—H3A3	109.5
O24—W1—O25	84.7 (3)	H3A1—C3A—H3A3	109.5
O19—W1—O25	89.1 (3)	H3A2—C3A—H3A3	109.5
O1—W1—O49	173.4 (3)	S2A—C4A—H4A1	109.5
O57—W1—O49	83.9 (3)	S2A—C4A—H4A2	109.5
O24—W1—O49	83.5 (3)	H4A1—C4A—H4A2	109.5
O19—W1—O49	73.6 (3)	S2A—C4A—H4A3	109.5
O25—W1—O49	80.8 (3)	H4A1—C4A—H4A3	109.5
O2—W2—O20	102.5 (4)	H4A2—C4A—H4A3	109.5
O2—W2—O58	99.3 (4)	S3A—O65—Zn1	142.5 (14)
O20—W2—O58	87.0 (3)	S3—O65—Zn1	122.8 (7)

O2—W2—O19	99.9 (4)	O65—S3—C5	104.9 (10)
O20—W2—O19	157.5 (3)	O65—S3—C6	105.6 (8)
O58—W2—O19	89.5 (3)	C5—S3—C6	101.6 (12)
O2—W2—O26	97.3 (4)	S3—C5—H5A	109.5
O20—W2—O26	86.9 (3)	S3—C5—H5B	109.5
O58—W2—O26	163.2 (3)	H5A—C5—H5B	109.5
O19—W2—O26	90.2 (4)	S3—C5—H5C	109.5
O2—W2—O49	173.3 (3)	H5A—C5—H5C	109.5
O20—W2—O49	84.1 (3)	H5B—C5—H5C	109.5
O58—W2—O49	81.8 (3)	S3—C6—H6A	109.5
O19—W2—O49	73.5 (3)	S3—C6—H6B	109.5
O26—W2—O49	82.0 (3)	H6A—C6—H6B	109.5
O3—W3—O59	98.7 (4)	S3—C6—H6C	109.5
O3—W3—O20	101.6 (4)	H6A—C6—H6C	109.5
O59—W3—O20	88.4 (3)	H6B—C6—H6C	109.5
O3—W3—O21	100.2 (3)	O65—S3A—C6A	120 (2)
O59—W3—O21	91.5 (3)	O65—S3A—C5A	108.7 (18)
O20—W3—O21	157.9 (3)	C6A—S3A—C5A	108.9 (18)
O3—W3—O27	97.6 (4)	S3A—C5A—H5A1	109.5
O59—W3—O27	163.4 (3)	S3A—C5A—H5A2	109.5
O20—W3—O27	85.3 (3)	H5A1—C5A—H5A2	109.5
O21—W3—O27	88.7 (3)	S3A—C5A—H5A3	109.5
O3—W3—O50	173.9 (3)	H5A1—C5A—H5A3	109.5
O59—W3—O50	83.2 (3)	H5A2—C5A—H5A3	109.5
O20—W3—O50	84.1 (3)	S3A—C6A—H6A1	109.5
O21—W3—O50	73.9 (3)	S3A—C6A—H6A2	109.5
O27—W3—O50	80.9 (3)	H6A1—C6A—H6A2	109.5
O4—W4—O22	102.7 (3)	S3A—C6A—H6A3	109.5
O4—W4—O60	98.7 (4)	H6A1—C6A—H6A3	109.5
O22—W4—O60	88.9 (3)	H6A2—C6A—H6A3	109.5
O4—W4—O28	97.6 (4)	S4—O66—Zn1	118.3 (5)
O22—W4—O28	85.8 (3)	O66—S4—C7	104.6 (9)
O60—W4—O28	163.6 (3)	O66—S4—C8	103.1 (10)
O4—W4—O21	100.5 (3)	C7—S4—C8	95.3 (12)
O22—W4—O21	156.7 (3)	S4—C7—H7A	109.5
O60—W4—O21	89.3 (3)	S4—C7—H7B	109.5
O28—W4—O21	89.5 (3)	H7A—C7—H7B	109.5
O4—W4—O50	173.3 (3)	S4—C7—H7C	109.5
O22—W4—O50	83.9 (3)	H7A—C7—H7C	109.5
O60—W4—O50	82.9 (3)	H7B—C7—H7C	109.5
O28—W4—O50	81.1 (3)	S4—C8—H8A	109.5
O21—W4—O50	72.9 (3)	S4—C8—H8B	109.5
O5—W5—O22	102.6 (4)	H8A—C8—H8B	109.5
O5—W5—O61	98.7 (4)	S4—C8—H8C	109.5
O22—W5—O61	88.3 (3)	H8A—C8—H8C	109.5
O5—W5—O23	100.4 (4)	H8B—C8—H8C	109.5
O22—W5—O23	156.8 (3)	S5—O67—Zn1	125.7 (5)
O61—W5—O23	91.8 (3)	O67—S5—C10	104.3 (9)

O5—W5—O29	97.1 (4)	O67—S5—C9	105.6 (7)
O22—W5—O29	84.9 (3)	C10—S5—C9	97.9 (10)
O61—W5—O29	163.8 (3)	S5—C9—H9A	109.5
O23—W5—O29	88.8 (3)	S5—C9—H9B	109.5
O5—W5—O51	173.3 (3)	H9A—C9—H9B	109.5
O22—W5—O51	83.8 (3)	S5—C9—H9C	109.5
O61—W5—O51	83.6 (3)	H9A—C9—H9C	109.5
O23—W5—O51	73.2 (3)	H9B—C9—H9C	109.5
O29—W5—O51	81.1 (3)	S5—C10—H10A	109.5
O6—W6—O24	102.9 (4)	S5—C10—H10B	109.5
O6—W6—O62	98.1 (4)	H10A—C10—H10B	109.5
O24—W6—O62	88.5 (3)	S5—C10—H10C	109.5
O6—W6—O23	100.5 (4)	H10A—C10—H10C	109.5
O24—W6—O23	156.6 (3)	H10B—C10—H10C	109.5
O62—W6—O23	89.2 (3)	S6—O68—Zn1	132.7 (7)
O6—W6—O30	98.1 (4)	O68—S6—C11	106.8 (7)
O24—W6—O30	86.2 (3)	O68—S6—C12	101.7 (10)
O62—W6—O30	163.8 (3)	C11—S6—C12	96.7 (11)
O23—W6—O30	89.6 (3)	S6—C11—H11A	109.5
O6—W6—O51	173.7 (3)	S6—C11—H11B	109.5
O24—W6—O51	83.4 (3)	H11A—C11—H11B	109.5
O62—W6—O51	82.5 (3)	S6—C11—H11C	109.5
O23—W6—O51	73.2 (3)	H11A—C11—H11C	109.5
O30—W6—O51	81.7 (3)	H11B—C11—H11C	109.5
O7—W7—O25	102.5 (4)	S6—C12—H12A	109.5
O7—W7—O30	101.9 (4)	S6—C12—H12B	109.5
O25—W7—O30	86.2 (3)	H12A—C12—H12B	109.5
O7—W7—O31	100.3 (4)	S6—C12—H12C	109.5
O25—W7—O31	90.4 (3)	H12A—C12—H12C	109.5
O30—W7—O31	157.7 (3)	H12B—C12—H12C	109.5
O7—W7—O33	100.6 (4)	O69—Zn2—O73	94.5 (5)
O25—W7—O33	156.8 (3)	O69—Zn2—O72	94.0 (4)
O30—W7—O33	88.0 (3)	O73—Zn2—O72	90.7 (4)
O31—W7—O33	86.6 (3)	O69—Zn2—O71	92.3 (5)
O7—W7—O52	170.8 (3)	O73—Zn2—O71	173.3 (4)
O25—W7—O52	84.5 (3)	O72—Zn2—O71	89.0 (4)
O30—W7—O52	84.3 (3)	O69—Zn2—O70	86.3 (4)
O31—W7—O52	73.4 (3)	O73—Zn2—O70	93.5 (4)
O33—W7—O52	72.6 (3)	O72—Zn2—O70	175.8 (4)
O8—W8—O27	102.2 (4)	O71—Zn2—O70	86.7 (4)
O8—W8—O26	103.3 (4)	O69—Zn2—O9	174.7 (4)
O27—W8—O26	86.5 (3)	O73—Zn2—O9	86.2 (4)
O8—W8—O32	99.8 (4)	O72—Zn2—O9	91.3 (3)
O27—W8—O32	90.0 (3)	O71—Zn2—O9	87.1 (4)
O26—W8—O32	156.9 (3)	O70—Zn2—O9	88.3 (3)
O8—W8—O31	100.9 (4)	Zn2—O69—H169	140.4
O27—W8—O31	156.9 (3)	Zn2—O69—H269	108.9
O26—W8—O31	87.6 (4)	H169—O69—H269	107.7

O32—W8—O31	86.8 (3)	C13—O70—Zn2	123.7 (8)
O8—W8—O52	170.4 (4)	C13—O70—HO70	108.9
O27—W8—O52	84.4 (3)	Zn2—O70—HO70	120.8
O26—W8—O52	84.0 (3)	O70—C13—C14	112.0 (13)
O32—W8—O52	73.0 (3)	O70—C13—H13A	109.2
O31—W8—O52	72.7 (3)	C14—C13—H13A	109.2
O9—W9—O29	102.8 (3)	O70—C13—H13B	109.2
O9—W9—O28	103.6 (3)	C14—C13—H13B	109.2
O29—W9—O28	86.6 (3)	H13A—C13—H13B	107.9
O9—W9—O33	100.1 (4)	C13—C14—H14A	109.5
O29—W9—O33	89.4 (3)	C13—C14—H14B	109.5
O28—W9—O33	156.3 (3)	H14A—C14—H14B	109.5
O9—W9—O32	99.7 (4)	C13—C14—H14C	109.5
O29—W9—O32	157.5 (3)	H14A—C14—H14C	109.5
O28—W9—O32	87.6 (3)	H14B—C14—H14C	109.5
O33—W9—O32	87.2 (3)	S8—O71—Zn2	118.3 (5)
O9—W9—O52	170.1 (3)	O71—S8—C15	103.2 (7)
O29—W9—O52	84.4 (3)	O71—S8—C16	108.5 (8)
O28—W9—O52	83.4 (3)	C15—S8—C16	97.3 (8)
O33—W9—O52	73.0 (3)	S8—C15—H15A	109.5
O32—W9—O52	73.3 (3)	S8—C15—H15B	109.5
O10—W10—O39	102.3 (4)	H15A—C15—H15B	109.5
O10—W10—O57	98.5 (4)	S8—C15—H15C	109.5
O39—W10—O57	88.7 (4)	H15A—C15—H15C	109.5
O10—W10—O34	100.4 (4)	H15B—C15—H15C	109.5
O39—W10—O34	157.2 (3)	S8—C16—H16A	109.5
O57—W10—O34	89.8 (4)	S8—C16—H16B	109.5
O10—W10—O40	98.0 (4)	H16A—C16—H16B	109.5
O39—W10—O40	86.1 (3)	S8—C16—H16C	109.5
O57—W10—O40	163.4 (3)	H16A—C16—H16C	109.5
O34—W10—O40	88.9 (3)	H16B—C16—H16C	109.5
O10—W10—O53	173.4 (4)	S9A—O72—Zn2	143.6 (14)
O39—W10—O53	84.1 (3)	S9—O72—Zn2	124.3 (6)
O57—W10—O53	82.8 (3)	O72—S9—C17	105.4 (8)
O34—W10—O53	73.1 (3)	O72—S9—C18	104.4 (8)
O40—W10—O53	81.0 (3)	C17—S9—C18	100.6 (10)
O11—W11—O58	98.9 (4)	S9—C17—H17A	109.5
O11—W11—O34	100.0 (4)	S9—C17—H17B	109.5
O58—W11—O34	93.1 (4)	H17A—C17—H17B	109.5
O11—W11—O35	101.7 (4)	S9—C17—H17C	109.5
O58—W11—O35	87.7 (3)	H17A—C17—H17C	109.5
O34—W11—O35	157.9 (3)	H17B—C17—H17C	109.5
O11—W11—O41	96.7 (4)	S9—C18—H18A	109.5
O58—W11—O41	163.7 (3)	S9—C18—H18B	109.5
O34—W11—O41	88.8 (3)	H18A—C18—H18B	109.5
O35—W11—O41	84.5 (3)	S9—C18—H18C	109.5
O11—W11—O53	173.5 (3)	H18A—C18—H18C	109.5
O58—W11—O53	83.9 (3)	H18B—C18—H18C	109.5

O34—W11—O53	73.9 (3)	O72—S9A—C17A	107.3 (14)
O35—W11—O53	84.3 (3)	O72—S9A—C18A	108.6 (18)
O41—W11—O53	81.1 (3)	C17A—S9A—C18A	102.0 (15)
O12—W12—O35	101.8 (3)	S9A—C17A—H17D	109.5
O12—W12—O36	100.6 (3)	S9A—C17A—H17E	109.5
O35—W12—O36	157.5 (3)	H17D—C17A—H17E	109.5
O12—W12—O42	97.9 (4)	S9A—C17A—H17F	109.5
O35—W12—O42	86.9 (3)	H17D—C17A—H17F	109.5
O36—W12—O42	90.3 (3)	H17E—C17A—H17F	109.5
O12—W12—O59	98.5 (4)	S9A—C18A—H18D	109.5
O35—W12—O59	88.0 (3)	S9A—C18A—H18E	109.5
O36—W12—O59	88.4 (3)	H18D—C18A—H18E	109.5
O42—W12—O59	163.6 (3)	S9A—C18A—H18F	109.5
O12—W12—O54	174.1 (3)	H18D—C18A—H18F	109.5
O35—W12—O54	84.1 (3)	H18E—C18A—H18F	109.5
O36—W12—O54	73.4 (3)	S10—O73—Zn2	129.8 (6)
O42—W12—O54	82.0 (3)	O73—S10—C19	106.9 (8)
O59—W12—O54	81.9 (3)	O73—S10—C20	104.1 (10)
O13—W13—O60	98.3 (3)	C19—S10—C20	93.0 (10)
O13—W13—O37	102.5 (4)	S10—C19—H19A	109.5
O60—W13—O37	88.4 (3)	S10—C19—H19B	109.5
O13—W13—O36	100.1 (4)	H19A—C19—H19B	109.5
O60—W13—O36	90.4 (3)	S10—C19—H19C	109.5
O37—W13—O36	157.3 (3)	H19A—C19—H19C	109.5
O13—W13—O43	97.0 (4)	H19B—C19—H19C	109.5
O60—W13—O43	164.5 (3)	S10—C20—H20A	109.5
O37—W13—O43	85.8 (3)	S10—C20—H20B	109.5
O36—W13—O43	89.5 (3)	H20A—C20—H20B	109.5
O13—W13—O54	172.5 (3)	S10—C20—H20C	109.5
O60—W13—O54	83.5 (3)	H20A—C20—H20C	109.5
O37—W13—O54	84.7 (3)	H20B—C20—H20C	109.5
O36—W13—O54	72.6 (3)	S11A—O74—Zn3	146.5 (14)
O43—W13—O54	81.7 (3)	S11—O74—Zn3	130.2 (7)
O14—W14—O61	97.4 (4)	O78—Zn3—O75	177.5 (4)
O14—W14—O37	102.5 (4)	O78—Zn3—O77	92.4 (4)
O61—W14—O37	87.7 (3)	O75—Zn3—O77	90.1 (4)
O14—W14—O44	98.9 (4)	O78—Zn3—O74	87.7 (4)
O61—W14—O44	163.6 (3)	O75—Zn3—O74	89.8 (4)
O37—W14—O44	87.2 (3)	O77—Zn3—O74	172.5 (5)
O14—W14—O38	99.8 (4)	O78—Zn3—O76	88.6 (4)
O61—W14—O38	89.1 (3)	O75—Zn3—O76	91.0 (4)
O37—W14—O38	157.7 (3)	O77—Zn3—O76	92.5 (5)
O44—W14—O38	89.8 (3)	O74—Zn3—O76	95.0 (5)
O14—W14—O55	172.9 (3)	O78—Zn3—O79	89.8 (4)
O61—W14—O55	81.7 (3)	O75—Zn3—O79	90.5 (3)
O37—W14—O55	84.5 (3)	O77—Zn3—O79	89.7 (4)
O44—W14—O55	82.3 (3)	O74—Zn3—O79	82.8 (4)
O38—W14—O55	73.2 (3)	O76—Zn3—O79	177.3 (4)

O15—W15—O62	98.7 (4)	O74—S11—C22	104.7 (7)
O15—W15—O38	100.1 (4)	O74—S11—C21	106.8 (7)
O62—W15—O38	91.9 (3)	C22—S11—C21	99.7 (8)
O15—W15—O39	102.3 (4)	S11—C21—H21A	109.5
O62—W15—O39	88.7 (3)	S11—C21—H21B	109.5
O38—W15—O39	157.3 (3)	H21A—C21—H21B	109.5
O15—W15—O45	96.9 (4)	S11—C21—H21C	109.5
O62—W15—O45	164.0 (3)	H21A—C21—H21C	109.5
O38—W15—O45	88.9 (3)	H21B—C21—H21C	109.5
O39—W15—O45	84.4 (3)	S11—C22—H22A	109.5
O15—W15—O55	173.4 (3)	S11—C22—H22B	109.5
O62—W15—O55	83.5 (3)	H22A—C22—H22B	109.5
O38—W15—O55	73.6 (3)	S11—C22—H22C	109.5
O39—W15—O55	84.0 (3)	H22A—C22—H22C	109.5
O45—W15—O55	81.4 (3)	H22B—C22—H22C	109.5
O16—W16—O45	101.9 (4)	O74—S11A—C21A	127 (2)
O16—W16—O40	102.3 (4)	O74—S11A—C22A	112.7 (19)
O45—W16—O40	86.1 (4)	C21A—S11A—C22A	103.9 (17)
O16—W16—O46	100.8 (4)	S11A—C21A—H21D	109.5
O45—W16—O46	157.4 (3)	S11A—C21A—H21E	109.5
O40—W16—O46	88.5 (4)	H21D—C21A—H21E	109.5
O16—W16—O48	101.3 (4)	S11A—C21A—H21F	109.5
O45—W16—O48	89.3 (4)	H21D—C21A—H21F	109.5
O40—W16—O48	156.3 (3)	H21E—C21A—H21F	109.5
O46—W16—O48	86.9 (3)	S11A—C22A—H22D	109.5
O16—W16—O56	171.2 (4)	S11A—C22A—H22E	109.5
O45—W16—O56	84.8 (3)	H22D—C22A—H22E	109.5
O40—W16—O56	83.6 (3)	S11A—C22A—H22F	109.5
O46—W16—O56	72.7 (3)	H22D—C22A—H22F	109.5
O48—W16—O56	72.8 (3)	H22E—C22A—H22F	109.5
O17—W17—O41	103.7 (4)	S12—O75—Zn3	122.5 (5)
O17—W17—O46	101.9 (4)	O75—S12—C23	103.5 (6)
O41—W17—O46	90.6 (3)	O75—S12—C24	103.7 (7)
O17—W17—O42	101.8 (4)	C23—S12—C24	97.8 (8)
O41—W17—O42	85.5 (3)	S12—C23—H23A	109.5
O46—W17—O42	156.3 (3)	S12—C23—H23B	109.5
O17—W17—O47	100.2 (4)	H23A—C23—H23B	109.5
O41—W17—O47	155.9 (4)	S12—C23—H23C	109.5
O46—W17—O47	87.1 (3)	H23A—C23—H23C	109.5
O42—W17—O47	87.1 (3)	H23B—C23—H23C	109.5
O17—W17—O56	171.2 (3)	S12—C24—H24A	109.5
O41—W17—O56	83.7 (3)	S12—C24—H24B	109.5
O46—W17—O56	73.0 (3)	H24A—C24—H24B	109.5
O42—W17—O56	83.4 (3)	S12—C24—H24C	109.5
O47—W17—O56	72.7 (3)	H24A—C24—H24C	109.5
O18—W18—O43	101.9 (4)	H24B—C24—H24C	109.5
O18—W18—O47	100.6 (4)	S13—O76—Zn3	144.4 (7)
O43—W18—O47	89.8 (3)	O76—S13—C25	99.4 (12)

O18—W18—O48	101.0 (4)	O76—S13—C26	107.4 (11)
O43—W18—O48	157.0 (3)	C25—S13—C26	95.3 (13)
O47—W18—O48	88.3 (3)	S13—C25—H25A	109.5
O18—W18—O44	102.9 (4)	S13—C25—H25B	109.5
O43—W18—O44	85.8 (3)	H25A—C25—H25B	109.5
O47—W18—O44	156.5 (3)	S13—C25—H25C	109.5
O48—W18—O44	87.0 (3)	H25A—C25—H25C	109.5
O18—W18—O56	171.0 (3)	H25B—C25—H25C	109.5
O43—W18—O56	84.6 (3)	S13—C26—H26A	109.5
O47—W18—O56	73.1 (3)	S13—C26—H26B	109.5
O48—W18—O56	72.9 (3)	H26A—C26—H26B	109.5
O44—W18—O56	83.6 (3)	S13—C26—H26C	109.5
O50—P1—O51	113.5 (4)	H26A—C26—H26C	109.5
O50—P1—O49	111.6 (4)	H26B—C26—H26C	109.5
O51—P1—O49	111.3 (4)	S14A—O77—Zn3	132.9 (11)
O50—P1—O52	106.7 (4)	S14—O77—Zn3	139.7 (7)
O51—P1—O52	106.3 (4)	O77—S14—C27	108.1 (10)
O49—P1—O52	107.0 (4)	O77—S14—C28	104.4 (9)
O55—P2—O54	111.8 (4)	C27—S14—C28	99.7 (13)
O55—P2—O53	111.3 (4)	S14—C27—H27A	109.5
O54—P2—O53	112.0 (4)	S14—C27—H27B	109.5
O55—P2—O56	107.7 (4)	H27A—C27—H27B	109.5
O54—P2—O56	106.8 (4)	S14—C27—H27C	109.5
O53—P2—O56	107.0 (4)	H27A—C27—H27C	109.5
W9—O9—Zn2	174.4 (5)	H27B—C27—H27C	109.5
W1—O19—W2	122.8 (4)	S14—C28—H28A	109.5
W3—O20—W2	151.5 (5)	S14—C28—H28B	109.5
W3—O21—W4	122.5 (3)	H28A—C28—H28B	109.5
W5—O22—W4	153.3 (4)	S14—C28—H28C	109.5
W6—O23—W5	123.2 (4)	H28A—C28—H28C	109.5
W6—O24—W1	153.2 (4)	H28B—C28—H28C	109.5
W7—O25—W1	152.0 (4)	O77—S14A—C28A	110.4 (14)
W8—O26—W2	150.0 (5)	O77—S14A—C27A	106.6 (14)
W8—O27—W3	151.8 (4)	C28A—S14A—C27A	98.0 (12)
W4—O28—W9	151.0 (4)	S14A—C27A—H27D	109.5
W9—O29—W5	151.0 (4)	S14A—C27A—H27E	109.5
W7—O30—W6	150.0 (5)	H27D—C27A—H27E	109.5
W7—O31—W8	122.8 (4)	S14A—C27A—H27F	109.5
W8—O32—W9	122.6 (4)	H27D—C27A—H27F	109.5
W9—O33—W7	123.2 (4)	H27E—C27A—H27F	109.5
W11—O34—W10	122.5 (4)	S14A—C28A—H28D	109.5
W12—O35—W11	151.7 (4)	S14A—C28A—H28E	109.5
W12—O36—W13	123.4 (4)	H28D—C28A—H28E	109.5
W13—O37—W14	150.6 (4)	S14A—C28A—H28F	109.5
W15—O38—W14	123.3 (4)	H28D—C28A—H28F	109.5
W10—O39—W15	152.6 (5)	H28E—C28A—H28F	109.5
W16—O40—W10	151.0 (4)	S15—O78—Zn3	124.1 (6)
W17—O41—W11	152.7 (4)	O78—S15—C30	106.9 (7)

W17—O42—W12	150.6 (4)	O78—S15—C29	104.2 (6)
W18—O43—W13	151.6 (5)	C30—S15—C29	97.7 (8)
W14—O44—W18	150.2 (4)	S15—C29—H29A	109.5
W16—O45—W15	151.3 (4)	S15—C29—H29B	109.5
W17—O46—W16	123.8 (4)	H29A—C29—H29B	109.5
W18—O47—W17	123.7 (4)	S15—C29—H29C	109.5
W18—O48—W16	123.7 (4)	H29A—C29—H29C	109.5
P1—O49—W2	127.8 (4)	H29B—C29—H29C	109.5
P1—O49—W1	128.7 (4)	S15—C30—H30A	109.5
W2—O49—W1	90.0 (2)	S15—C30—H30B	109.5
P1—O50—W3	129.7 (4)	H30A—C30—H30B	109.5
P1—O50—W4	127.4 (4)	S15—C30—H30C	109.5
W3—O50—W4	90.5 (2)	H30A—C30—H30C	109.5
P1—O51—W5	128.2 (4)	H30B—C30—H30C	109.5
P1—O51—W6	129.0 (4)	S16—O79—Zn3	122.0 (6)
W5—O51—W6	90.2 (2)	O79—S16—C31	101.7 (7)
P1—O52—W9	124.6 (4)	O79—S16—C32	105.0 (6)
P1—O52—W7	124.5 (4)	C31—S16—C32	99.5 (10)
W9—O52—W7	91.2 (3)	S16—C31—H31A	109.5
P1—O52—W8	124.2 (4)	S16—C31—H31B	109.5
W9—O52—W8	91.1 (2)	H31A—C31—H31B	109.5
W7—O52—W8	91.0 (2)	S16—C31—H31C	109.5
P2—O53—W11	128.5 (4)	H31A—C31—H31C	109.5
P2—O53—W10	128.3 (4)	H31B—C31—H31C	109.5
W11—O53—W10	90.2 (2)	S16—C32—H32A	109.5
P2—O54—W12	127.9 (4)	S16—C32—H32B	109.5
P2—O54—W13	128.2 (4)	H32A—C32—H32B	109.5
W12—O54—W13	90.4 (2)	S16—C32—H32C	109.5
P2—O55—W15	128.6 (4)	H32A—C32—H32C	109.5
P2—O55—W14	127.5 (4)	H32B—C32—H32C	109.5
W15—O55—W14	89.8 (2)	O81—S18—C34	103.7 (9)
P2—O56—W16	124.6 (4)	O81—S18—C33	106.0 (10)
P2—O56—W17	125.1 (4)	C34—S18—C33	95.4 (11)
W16—O56—W17	90.6 (3)	S18—C33—H33A	109.5
P2—O56—W18	124.9 (4)	S18—C33—H33B	109.5
W16—O56—W18	90.6 (3)	H33A—C33—H33B	109.5
W17—O56—W18	90.5 (3)	S18—C33—H33C	109.5
W1—O57—W10	163.0 (5)	H33A—C33—H33C	109.5
W11—O58—W2	164.7 (5)	H33B—C33—H33C	109.5
W3—O59—W12	163.1 (4)	S18—C34—H34A	109.5
W13—O60—W4	162.6 (4)	S18—C34—H34B	109.5
W14—O61—W5	163.6 (4)	H34A—C34—H34B	109.5
W15—O62—W6	163.4 (4)	S18—C34—H34C	109.5
O65—Zn1—O66	93.9 (4)	H34A—C34—H34C	109.5
O65—Zn1—O63	91.1 (4)	H34B—C34—H34C	109.5
O66—Zn1—O63	174.7 (4)	C35—S19—C36	104.2 (16)
O65—Zn1—O64	87.3 (5)	C35—S19—O82	97.8 (12)
O66—Zn1—O64	93.8 (4)	C36—S19—O82	101.8 (17)

O63—Zn1—O64	88.0 (4)	S19—C35—H35A	109.5
O65—Zn1—O67	88.6 (4)	S19—C35—H35B	109.5
O66—Zn1—O67	88.0 (4)	H35A—C35—H35B	109.5
O63—Zn1—O67	90.6 (4)	S19—C35—H35C	109.5
O64—Zn1—O67	175.6 (5)	H35A—C35—H35C	109.5
O65—Zn1—O68	174.4 (4)	H35B—C35—H35C	109.5
O66—Zn1—O68	84.2 (4)	S19—C36—H36A	109.5
O63—Zn1—O68	90.6 (4)	S19—C36—H36B	109.5
O64—Zn1—O68	98.1 (5)	H36A—C36—H36B	109.5
O67—Zn1—O68	86.0 (4)	S19—C36—H36C	109.5
S1—O63—Zn1	120.5 (5)	H36A—C36—H36C	109.5
O63—S1—C1	105.6 (7)	H36B—C36—H36C	109.5
O63—S1—C2	103.5 (7)	C35A—S19A—C36A	106 (2)
C1—S1—C2	97.4 (8)	C35A—S19A—O82	107.5 (17)
S1—C1—H1A	109.5	C36A—S19A—O82	104.8 (18)
S1—C1—H1B	109.5	S19A—C35A—H35D	109.5
H1A—C1—H1B	109.5	S19A—C35A—H35E	109.5
S1—C1—H1C	109.5	H35D—C35A—H35E	109.5
H1A—C1—H1C	109.5	S19A—C35A—H35F	109.5
H1B—C1—H1C	109.5	H35D—C35A—H35F	109.5
S1—C2—H2A	109.5	H35E—C35A—H35F	109.5
S1—C2—H2B	109.5	S19A—C36A—H36D	109.5
H2A—C2—H2B	109.5	S19A—C36A—H36E	109.5
S1—C2—H2C	109.5	H36D—C36A—H36E	109.5
H2A—C2—H2C	109.5	S19A—C36A—H36F	109.5
H2B—C2—H2C	109.5	H36D—C36A—H36F	109.5
S2A—O64—Zn1	146.5 (13)	H36E—C36A—H36F	109.5
S2—O64—Zn1	121.1 (8)	C38—C37—H37A	109.5
O64—S2—C4	105.7 (8)	C38—C37—H37B	109.5
O64—S2—C3	106.1 (8)	H37A—C37—H37B	109.5
C4—S2—C3	97.5 (10)	C38—C37—H37C	109.5
S2—C3—H3A	109.5	H37A—C37—H37C	109.5
S2—C3—H3B	109.5	H37B—C37—H37C	109.5
H3A—C3—H3B	109.5	C37—C38—O83	104 (4)
S2—C3—H3C	109.5	C37—C38—H38A	110.9
H3A—C3—H3C	109.5	O83—C38—H38A	110.9
H3B—C3—H3C	109.5	C37—C38—H38B	110.9
S2—C4—H4A	109.5	O83—C38—H38B	110.9
S2—C4—H4B	109.5	H38A—C38—H38B	109.0
H4A—C4—H4B	109.5	C38—O83—H83	109.5
S2—C4—H4C	109.5	H11W—O1W—H21W	107.7
H4A—C4—H4C	109.5	H12W—O2W—H22W	107.7

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H11*W*···O79	0.85	2.12	2.934 (19)	162
O1*W*—H21*W*···O3^{i}	0.85	2.18	3.005 (19)	165

O2*W*—H12*W*···S13	0.85	2.73	3.30 (2)	125
O2*W*—H12*W*···O76	0.85	1.87	2.63 (2)	147
O2*W*—H22*W*···O17^{ii}	0.85	1.97	2.72 (3)	146
O69—H269···O81^{iii}	0.85	1.96	2.696 (16)	144
O70—H*O*70···O81^{iii}	0.85	2.18	2.856 (15)	136
C2—H2*A*···O8^{i}	0.97	2.49	3.313 (19)	143
C2—H2*C*···O16^{ii}	0.97	2.50	3.330 (19)	144
C3—H3*B*···O63	0.97	2.57	3.31 (2)	133
C9—H9*C*···O11^{iv}	0.97	2.55	3.48 (2)	161
C10—H10*C*···O8^{i}	0.97	2.55	3.36 (2)	141
C11—H11*A*···O1^{v}	0.97	2.57	3.49 (2)	160
C13—H13*A*···O32	0.98	2.46	3.345 (16)	150
C15—H15*A*···O4	0.97	2.36	3.05 (2)	127
C15—H15*C*···O36^{vi}	0.97	2.57	3.531 (19)	171
C16—H16*B*···O12^{vi}	0.97	2.58	3.39 (2)	142
C17—H17*C*···O73	0.97	2.55	3.27 (2)	131
C19—H19*A*···O33	0.97	2.45	3.36 (2)	158
C23—H23*A*···O21^{i}	0.97	2.39	3.357 (17)	176
C24—H24*A*···O32^{i}	0.97	2.57	3.477 (19)	156
C26—H26*C*···O75	0.97	2.58	3.31 (3)	132
C27—H27*A*···O34^{iv}	0.97	2.40	3.17 (2)	136
C27—H27*B*···O17^{ii}	0.97	2.42	3.38 (3)	172
C29—H29*A*···O7^{vii}	0.97	2.45	3.279 (19)	143
C30—H30*B*···O74	0.97	2.58	3.192 (18)	121
C30—H30*C*···O1^{iv}	0.97	2.52	3.449 (16)	159
C31—H31*A*···O19^{iv}	0.97	2.56	3.195 (17)	123
C32—H32*A*···O2^{iv}	0.97	2.53	3.365 (18)	144
C33—H33*A*···O43^{viii}	0.97	2.58	3.50 (2)	159
C37—H37*A*···S13	0.97	2.80	3.46 (2)	126
C37—H37*A*···O76	0.97	2.02	2.93 (2)	154

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