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[5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]zinc(II) dichloromethane tetrasolvate

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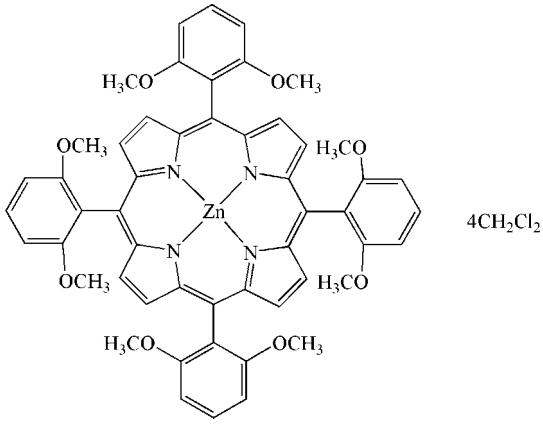
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.087; data-to-parameter ratio = 19.0.

The crystal structure, electronic spectroscopy and ^{1}H NMR data for the title compound, $[Zn(C_{52}H_{44}N_4O_8)]\cdot 4CH_2Cl_2$, are reported. The asymmetric unit consists of 0.5 zinc–porphyrin and two molecules of dichloromethane. The zinc ion is at a crystallographic inversion center and is four-coordinate with a planar porphyrin ligand.

Related literature

For details of the synthesis, see: Tsuchida, *et al.* (1990). For related *ortho*-substituted porphyrins, see: Bhryappa *et al.* (1997) For related literature, see: Allen (2002); Bruno *et al.* (2004); Rothemund & Menotti (1948); Suslick *et al.* (2005); Wagner *et al.* (1994).



Experimental

Crystal data

$[Zn(C_{52}H_{44}N_4O_8)]\cdot 4CH_2Cl_2$
M_r = 1257.99
Monoclinic, $P2_1/n$
a = 13.5090 (5) Å
b = 15.0743 (6) Å
c = 14.1788 (4) Å
β = 110.547 (1)°
V = 2703.67 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 100 (2) K
0.38 × 0.15 × 0.15 mm

Data collection

Bruker X8-APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick,2006)
T_{min} = 0.726, T_{max} = 0.874
63198 measured reflections
6691 independent reflections
5979 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.087
S = 1.05
6691 reflections
353 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2* and *SAINT* (Bruker, 2006); data reduction: *SAINT* and *XPREP* (Sheldrick, 2003); program(s) used to solve structure: *XS* (Sheldrick, 2001); program(s) used to refine structure: *XL* (Sheldrick, 2001); molecular graphics: *XP* (Sheldrick, 1998); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2062).

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supplementary materials

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[5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]zinc(II) dichloromethane tetrasolvate

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Comment

ortho-Functionalized porphyrins have generated interest for a variety of reasons. While *ortho* functionalization can prevent aggregation and unwanted reactions (Wagner *et al.*, 1994), Suslick used the title compound as a starting material for the construction of porous molecular solids (Suslick, 2005). As part of our continued investigations into the active site of hydroxylamine oxidoreductase (HAO) in *Nitrosomonas europea*, we report the solid state structure of tetra(2',6'-dimethoxyphenyl) porphyrin complexed with zinc. The compound is of interest as a non redox active control model of the active site of HAO. The characterized metalloporphyrin is stable to both air and moisture in both the solid and solution environments.

The compound is prepared by the reaction of zinc acetate with the ligand in refluxing glacial acetic acid. After purification by column chromatography, zinc tetra (2',6'-dimethoxyphenyl) porphyrin was dissolved in dichloromethane and layered with hexanes. This yielded crystals suitable for X-ray diffraction. The crystallographically determined structure is shown in Figure 1. The asymmetric unit consists of 0.5 zinc porphyrin and 2 molecules of dichloromethane. The zinc ion is at a crystallographic inversion center and is four coordinate with a planar porphyrin ligand. The nitrogen core is flat with Zn—N bond lengths of 2.0324 (13) Å and 2.0368 (13) Å which is slightly shorter than the median Zn—N bond distance of 2.046 Å for zinc porphyrins found in a search of the CSD (Allen, 2002). A closely related molecule, zinc tetra (2',6'-dihydroxyphenyl)porphyrin Zn[T(2',6'-DHP)P](EtOAc)$_2$ has a slightly longer average Zn—N bond distance of 2.043 Å in comparison to the title compound (Bhryappa, 1997). The ether C—O bonds are asymmetric, shorter to the aryl group, and longer to the methyl group. The Ar—O average bond distance is 1.366 (2) Å, comparable to the 1.366 (17) Å distance found from *MOGUL* (Bruno *et al.*, 2004). The average Me—O length is 1.428 (2) Å, which is consistent with 1.42 (4) Å found from *MOGUL*. Further studies are underway to examine the structural and solution properties of chloro iron (III) tetra (2',6'- dimethoxyphenyl) porphyrin and other metallo derivatives of tetra (2', 6'- dihydroxoxyphenyl) porphyrins.

Experimental

The ligand, 5,10,15,20 Tetra (2',6'-dimethoxyphenyl) porphyrin [(H_2T-2',6'- DMP)P] was synthesized following literature methods (Tsuchida *et al.*, 1990). Standard porphyrin metal insertion methods were used to obtain the title compound (Rothemund & Menotti, 1948). H_2T(2',6'-DMP)P (70 mg, 8.2×10^{-5} mol) was dissolved in glacial acetic acid (10 ml). Zinc acetate (180 mg, 8.2×10^{-4} mol) was added after all of the ligand dissolved and then the solution was refluxed at 100–130 °C for one h. The solvent was removed by vacuum filtration and the crystals were rinsed three times with water. The resulting purple crystals were dissolved in dichloromethane and the solution was chromatographed on a dry alumina column using dichloromethane as the eluent. (67% Yield); R_f (Alumina, DCM) 0.36; I.*R*·(KBr): 2933, 1431, 1335, 1249 [ν_{as} (C—O—C)], 1110, and 998 [ν (C—H)] cm-1; λ_{max}(DCM): 419, 546, and 579 nm; ε: 4.1×10^5, 7.1×10^3, and 6.6×10^2 $cm^{-1}M^{-1}$. ^{1}HNMR($CDCl_3$): 3.5(–OMe), 7.0–7.5(aromatic), and 8.8(pyrrole) p.p.m.;

Refinement

Hydrogen atoms were placed at calculated geometries and allowed to ride on the position of the parent atom. Parameters for thermal motion were set to 1.2× the equivalent isotropic U of the parent atom, 1.5× for methyl H atoms.

Figures

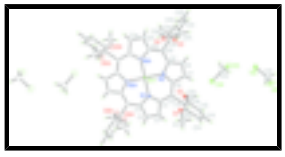

Fig. 1. Thermal ellipsoid plot showing the title compound and the dichloromethane of solvation. Zn1 is at a crystallographic center of symmetry. Symmetry equivalent atoms are shown with open ellipsoids. Ellipsoids are drawn at 50% probability.

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Crystal data

$[Zn(C_{52}H_{44}N_4O_8)]\cdot 4CH_2Cl_2$	F_{000} = 1292
M_r = 1257.99	D_x = 1.545 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7854 reflections
a = 13.5090 (5) Å	θ = 2.7–30.1°
b = 15.0743 (6) Å	μ = 0.91 mm^{-1}
c = 14.1788 (4) Å	T = 100 (2) K
β = 110.547 (1)°	Needle, translucent dark red
V = 2703.67 (17) Å^3	0.38 × 0.15 × 0.15 mm
Z = 2	

Data collection

Bruker X8-APEXII CCD diffractometer	6691 independent reflections
Monochromator: graphite	5979 reflections with $I > 2\sigma(I)$
Detector resolution: 8.33 pixels mm^{-1}	R_{int} = 0.029
T = 100(2) K	θ_{max} = 28.3°
φ and ω scans	θ_{min} = 1.8°
Absorption correction: multi-scan (SADABS; Sheldrick,2006)	h = −17→18
T_{min} = 0.726, T_{max} = 0.874	k = −20→19
63198 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.087$	$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 3.1885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
6691 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
353 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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. The asymmetric unit contains 1/2 Zn porphyrin and 2 molecules of dichloromethane. Zn is at a crystallographic inversion center.

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 $F^2 > 2\sigma(F^2)$ 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	0.0000	0.0000	0.5000	0.00956 (7)
N1	0.06157 (10)	0.05965 (9)	0.63681 (10)	0.0104 (3)
N2	0.12358 (10)	0.04630 (9)	0.46349 (10)	0.0102 (3)
O1	0.22057 (10)	0.31144 (8)	0.63177 (10)	0.0190 (3)
O2	0.41183 (10)	0.04560 (9)	0.71699 (10)	0.0192 (3)
O3	0.08075 (10)	0.09141 (8)	0.14607 (9)	0.0179 (3)
O4	0.16191 (10)	−0.18907 (8)	0.29078 (10)	0.0189 (3)
C1	0.01573 (12)	0.06372 (11)	0.70917 (11)	0.0107 (3)
C2	0.08169 (13)	0.11473 (11)	0.79364 (12)	0.0134 (3)
H2	0.0681	0.1271	0.8537	0.016*
C3	0.16680 (13)	0.14180 (11)	0.77160 (12)	0.0133 (3)
H3	0.2244	0.1762	0.8134	0.016*
C4	0.15313 (12)	0.10831 (11)	0.67259 (12)	0.0108 (3)
C5	0.22122 (12)	0.12685 (11)	0.62006 (12)	0.0108 (3)
C6	0.20585 (12)	0.09792 (10)	0.52196 (12)	0.0105 (3)
C7	0.27827 (13)	0.11453 (11)	0.46963 (12)	0.0121 (3)
H7	0.3404	0.1499	0.4928	0.015*
C8	0.24066 (12)	0.06996 (11)	0.38082 (12)	0.0120 (3)
H8	0.2723	0.0674	0.3307	0.014*
C9	0.14385 (12)	0.02726 (11)	0.37699 (11)	0.0102 (3)
C10	0.08105 (12)	−0.02571 (11)	0.29750 (11)	0.0106 (3)

C11	0.31887 (13)	0.17954 (11)	0.67393 (12)	0.0123 (3)
C12	0.31687 (13)	0.27228 (12)	0.67927 (12)	0.0147 (3)
C13	0.40815 (15)	0.32015 (13)	0.72980 (14)	0.0199 (4)
H13	0.4063	0.3831	0.7320	0.024*
C14	0.50133 (14)	0.27500 (13)	0.77673 (14)	0.0213 (4)
H14	0.5638	0.3076	0.8112	0.026*
C15	0.50609 (14)	0.18380 (13)	0.77490 (13)	0.0192 (4)
H15	0.5707	0.1537	0.8085	0.023*
C16	0.41458 (13)	0.13623 (12)	0.72301 (12)	0.0146 (3)
C17	0.21042 (17)	0.40184 (13)	0.65734 (16)	0.0265 (4)
H17A	0.2308	0.4073	0.7306	0.040*
H17B	0.1369	0.4210	0.6249	0.040*
H17C	0.2566	0.4392	0.6340	0.040*
C18	0.50458 (16)	0.00004 (14)	0.77865 (16)	0.0254 (4)
H18A	0.5637	0.0150	0.7567	0.038*
H18B	0.4921	−0.0641	0.7725	0.038*
H18C	0.5216	0.0180	0.8490	0.038*
C19	0.12417 (12)	−0.04911 (11)	0.21652 (12)	0.0121 (3)
C20	0.12455 (13)	0.01095 (12)	0.14153 (12)	0.0147 (3)
C21	0.16797 (14)	−0.01253 (13)	0.06877 (13)	0.0198 (4)
H21	0.1696	0.0289	0.0189	0.024*
C22	0.20830 (14)	−0.09676 (14)	0.07062 (13)	0.0214 (4)
H22	0.2378	−0.1128	0.0212	0.026*
C23	0.20713 (14)	−0.15862 (13)	0.14214 (13)	0.0190 (4)
H23	0.2340	−0.2167	0.1413	0.023*
C24	0.16557 (13)	−0.13396 (12)	0.21564 (12)	0.0148 (3)
C25	0.05780 (16)	0.14806 (13)	0.06016 (13)	0.0216 (4)
H25A	0.1239	0.1653	0.0513	0.032*
H25B	0.0211	0.2013	0.0703	0.032*
H25C	0.0127	0.1164	0.0000	0.032*
C26	0.19103 (17)	−0.27915 (13)	0.28487 (17)	0.0273 (4)
H26A	0.1446	−0.3051	0.2214	0.041*
H26B	0.1841	−0.3125	0.3415	0.041*
H26C	0.2645	−0.2818	0.2876	0.041*
C1S	0.96642 (18)	0.25153 (15)	0.52497 (18)	0.0351 (5)
H1S1	1.0297	0.2440	0.5059	0.042*
H1S2	0.9871	0.2394	0.5980	0.042*
Cl1	0.91977 (5)	0.36179 (4)	0.49994 (4)	0.04067 (15)
Cl2	0.86858 (4)	0.17594 (4)	0.45730 (4)	0.02907 (12)
C2S	0.63161 (17)	0.09694 (14)	0.48441 (16)	0.0266 (4)
H2S1	0.6132	0.0393	0.4491	0.032*
H2S2	0.7095	0.0996	0.5171	0.032*
Cl3	0.58869 (5)	0.18428 (3)	0.39562 (4)	0.03135 (12)
Cl4	0.57272 (4)	0.10412 (4)	0.57715 (4)	0.03187 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Zn1	0.00849 (12)	0.01227 (13)	0.00826 (12)	−0.00277 (9)	0.00337 (9)	−0.00213 (9)
N1	0.0093 (6)	0.0126 (6)	0.0098 (6)	−0.0015 (5)	0.0038 (5)	−0.0012 (5)
N2	0.0099 (6)	0.0113 (6)	0.0093 (6)	−0.0010 (5)	0.0035 (5)	−0.0013 (5)
O1	0.0168 (6)	0.0137 (6)	0.0265 (7)	−0.0005 (5)	0.0075 (5)	−0.0029 (5)
O2	0.0135 (6)	0.0170 (6)	0.0231 (6)	0.0001 (5)	0.0017 (5)	0.0011 (5)
O3	0.0250 (7)	0.0171 (6)	0.0132 (5)	0.0007 (5)	0.0089 (5)	0.0030 (5)
O4	0.0234 (7)	0.0150 (6)	0.0203 (6)	0.0047 (5)	0.0101 (5)	0.0014 (5)
C1	0.0116 (7)	0.0115 (7)	0.0090 (7)	−0.0005 (6)	0.0035 (6)	−0.0009 (6)
C2	0.0130 (8)	0.0164 (8)	0.0105 (7)	−0.0023 (6)	0.0037 (6)	−0.0027 (6)
C3	0.0130 (7)	0.0154 (8)	0.0104 (7)	−0.0033 (6)	0.0028 (6)	−0.0033 (6)
C4	0.0093 (7)	0.0118 (7)	0.0106 (7)	−0.0002 (6)	0.0025 (6)	−0.0011 (6)
C5	0.0090 (7)	0.0109 (7)	0.0118 (7)	−0.0007 (6)	0.0026 (6)	−0.0008 (6)
C6	0.0095 (7)	0.0101 (7)	0.0117 (7)	−0.0007 (6)	0.0036 (6)	0.0003 (6)
C7	0.0104 (7)	0.0134 (8)	0.0129 (7)	−0.0021 (6)	0.0047 (6)	0.0001 (6)
C8	0.0115 (7)	0.0126 (7)	0.0128 (7)	−0.0004 (6)	0.0055 (6)	0.0012 (6)
C9	0.0094 (7)	0.0112 (7)	0.0103 (7)	0.0010 (6)	0.0038 (5)	0.0011 (6)
C10	0.0111 (7)	0.0122 (7)	0.0090 (7)	0.0008 (6)	0.0042 (6)	0.0012 (6)
C11	0.0114 (7)	0.0163 (8)	0.0100 (7)	−0.0041 (6)	0.0047 (6)	−0.0025 (6)
C12	0.0145 (8)	0.0169 (8)	0.0147 (7)	−0.0033 (6)	0.0075 (6)	−0.0026 (6)
C13	0.0209 (9)	0.0179 (9)	0.0234 (9)	−0.0088 (7)	0.0109 (7)	−0.0066 (7)
C14	0.0164 (8)	0.0279 (10)	0.0196 (8)	−0.0119 (7)	0.0064 (7)	−0.0072 (7)
C15	0.0113 (8)	0.0283 (10)	0.0161 (8)	−0.0046 (7)	0.0023 (6)	−0.0001 (7)
C16	0.0137 (8)	0.0175 (8)	0.0130 (7)	−0.0038 (6)	0.0052 (6)	−0.0015 (6)
C17	0.0305 (11)	0.0169 (9)	0.0346 (11)	0.0022 (8)	0.0145 (9)	−0.0060 (8)
C18	0.0192 (9)	0.0251 (10)	0.0278 (10)	0.0042 (8)	0.0029 (8)	0.0066 (8)
C19	0.0097 (7)	0.0166 (8)	0.0101 (7)	−0.0024 (6)	0.0037 (6)	−0.0029 (6)
C20	0.0130 (8)	0.0192 (8)	0.0117 (7)	−0.0026 (6)	0.0042 (6)	−0.0016 (6)
C21	0.0174 (8)	0.0316 (10)	0.0124 (8)	−0.0035 (7)	0.0076 (7)	−0.0007 (7)
C22	0.0150 (8)	0.0365 (11)	0.0150 (8)	−0.0011 (7)	0.0084 (6)	−0.0071 (7)
C23	0.0124 (8)	0.0257 (9)	0.0181 (8)	0.0026 (7)	0.0044 (6)	−0.0076 (7)
C24	0.0111 (7)	0.0190 (8)	0.0134 (7)	−0.0016 (6)	0.0034 (6)	−0.0026 (6)
C25	0.0259 (10)	0.0227 (9)	0.0155 (8)	−0.0010 (7)	0.0063 (7)	0.0070 (7)
C26	0.0287 (10)	0.0185 (9)	0.0348 (11)	0.0086 (8)	0.0112 (9)	0.0018 (8)
C1S	0.0282 (11)	0.0283 (11)	0.0356 (11)	0.0042 (9)	−0.0050 (9)	−0.0046 (9)
Cl1	0.0454 (3)	0.0281 (3)	0.0340 (3)	0.0073 (2)	−0.0042 (2)	−0.0048 (2)
Cl2	0.0257 (2)	0.0308 (3)	0.0263 (2)	−0.00326 (19)	0.00364 (19)	0.00526 (19)
C2S	0.0322 (11)	0.0231 (10)	0.0276 (10)	0.0090 (8)	0.0142 (8)	0.0092 (8)
Cl3	0.0422 (3)	0.0211 (2)	0.0259 (2)	0.0049 (2)	0.0059 (2)	0.00504 (18)
Cl4	0.0307 (3)	0.0339 (3)	0.0367 (3)	0.0072 (2)	0.0189 (2)	0.0061 (2)

Geometric parameters (Å, °)

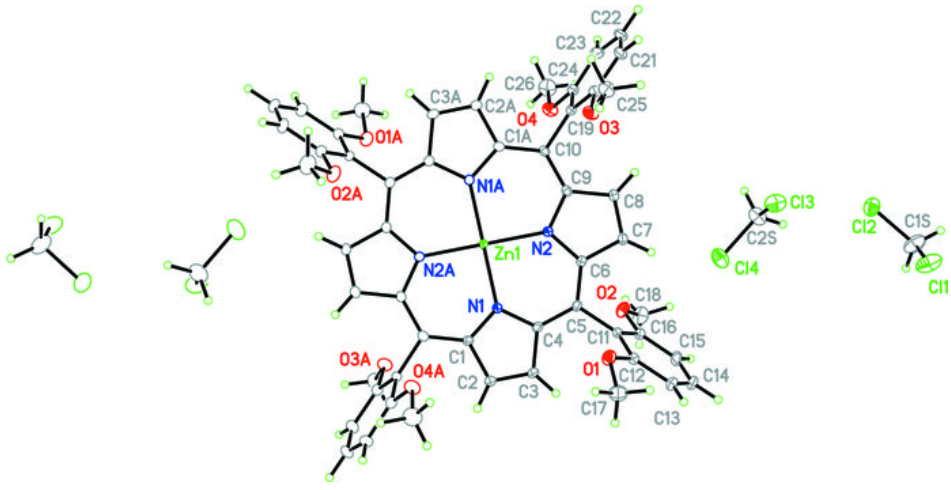
Zn1—N1	2.0324 (13)	C13—C14	1.379 (3)
Zn1—N1^{i}	2.0324 (13)	C13—H13	0.9500
Zn1—N2^{i}	2.0368 (13)	C14—C15	1.377 (3)
Zn1—N2	2.0368 (13)	C14—H14	0.9500
N1—C4	1.373 (2)	C15—C16	1.395 (2)
N1—C1	1.3733 (19)	C15—H15	0.9500
N2—C6	1.372 (2)	C17—H17A	0.9800

N2—C9	1.3775 (19)	C17—H17B	0.9800
O1—C12	1.371 (2)	C17—H17C	0.9800
O1—C17	1.429 (2)	C18—H18A	0.9800
O2—C16	1.368 (2)	C18—H18B	0.9800
O2—C18	1.427 (2)	C18—H18C	0.9800
O3—C20	1.361 (2)	C19—C24	1.398 (2)
O3—C25	1.430 (2)	C19—C20	1.398 (2)
O4—C24	1.365 (2)	C20—C21	1.399 (2)
O4—C26	1.424 (2)	C21—C22	1.378 (3)
C1—C10^{i}	1.400 (2)	C21—H21	0.9500
C1—C2	1.439 (2)	C22—C23	1.382 (3)
C2—C3	1.356 (2)	C22—H22	0.9500
C2—H2	0.9500	C23—C24	1.397 (2)
C3—C4	1.441 (2)	C23—H23	0.9500
C3—H3	0.9500	C25—H25A	0.9800
C4—C5	1.400 (2)	C25—H25B	0.9800
C5—C6	1.402 (2)	C25—H25C	0.9800
C5—C11	1.499 (2)	C26—H26A	0.9800
C6—C7	1.442 (2)	C26—H26B	0.9800
C7—C8	1.359 (2)	C26—H26C	0.9800
C7—H7	0.9500	C1S—Cl2	1.754 (2)
C8—C9	1.441 (2)	C1S—Cl1	1.769 (2)
C8—H8	0.9500	C1S—H1S1	0.9900
C9—C10	1.399 (2)	C1S—H1S2	0.9900
C10—C1^{i}	1.400 (2)	C2S—Cl4	1.763 (2)
C10—C19	1.501 (2)	C2S—Cl3	1.773 (2)
C11—C16	1.397 (2)	C2S—H2S1	0.9900
C11—C12	1.401 (2)	C2S—H2S2	0.9900
C12—C13	1.391 (2)		
N1—Zn1—N1^{i}	180.0	C14—C15—H15	120.5
N1—Zn1—N2^{i}	90.37 (5)	C16—C15—H15	120.5
N1^{i}—Zn1—N2^{i}	89.64 (5)	O2—C16—C15	123.07 (16)
N1—Zn1—N2	89.63 (5)	O2—C16—C11	115.82 (14)
N1^{i}—Zn1—N2	90.36 (5)	C15—C16—C11	121.11 (16)
N2^{i}—Zn1—N2	180.0	O1—C17—H17A	109.5
C4—N1—C1	106.50 (13)	O1—C17—H17B	109.5
C4—N1—Zn1	127.08 (10)	H17A—C17—H17B	109.5
C1—N1—Zn1	126.31 (11)	O1—C17—H17C	109.5
C6—N2—C9	106.52 (13)	H17A—C17—H17C	109.5
C6—N2—Zn1	127.11 (10)	H17B—C17—H17C	109.5
C9—N2—Zn1	126.28 (11)	O2—C18—H18A	109.5
C12—O1—C17	116.42 (14)	O2—C18—H18B	109.5
C16—O2—C18	116.32 (14)	H18A—C18—H18B	109.5
C20—O3—C25	117.38 (14)	O2—C18—H18C	109.5
C24—O4—C26	116.60 (14)	H18A—C18—H18C	109.5
N1—C1—C10^{i}	125.91 (14)	H18B—C18—H18C	109.5
N1—C1—C2	109.62 (14)	C24—C19—C20	118.53 (15)

C10^{i}—C1—C2	124.46 (14)	C24—C19—C10	119.07 (14)
C3—C2—C1	107.25 (14)	C20—C19—C10	122.40 (15)
C3—C2—H2	126.4	O3—C20—C19	115.06 (14)
C1—C2—H2	126.4	O3—C20—C21	124.19 (16)
C2—C3—C4	106.85 (14)	C19—C20—C21	120.75 (16)
C2—C3—H3	126.6	C22—C21—C20	118.96 (17)
C4—C3—H3	126.6	C22—C21—H21	120.5
N1—C4—C5	125.81 (14)	C20—C21—H21	120.5
N1—C4—C3	109.75 (13)	C21—C22—C23	121.96 (16)
C5—C4—C3	124.38 (15)	C21—C22—H22	119.0
C4—C5—C6	124.72 (15)	C23—C22—H22	119.0
C4—C5—C11	117.37 (14)	C22—C23—C24	118.64 (17)
C6—C5—C11	117.89 (14)	C22—C23—H23	120.7
N2—C6—C5	125.63 (14)	C24—C23—H23	120.7
N2—C6—C7	109.85 (13)	O4—C24—C23	123.67 (16)
C5—C6—C7	124.44 (15)	O4—C24—C19	115.19 (14)
C8—C7—C6	106.89 (14)	C23—C24—C19	121.14 (16)
C8—C7—H7	126.6	O3—C25—H25A	109.5
C6—C7—H7	126.6	O3—C25—H25B	109.5
C7—C8—C9	107.15 (14)	H25A—C25—H25B	109.5
C7—C8—H8	126.4	O3—C25—H25C	109.5
C9—C8—H8	126.4	H25A—C25—H25C	109.5
N2—C9—C10	125.63 (14)	H25B—C25—H25C	109.5
N2—C9—C8	109.55 (14)	O4—C26—H26A	109.5
C10—C9—C8	124.82 (14)	O4—C26—H26B	109.5
C9—C10—C1^{i}	125.18 (14)	H26A—C26—H26B	109.5
C9—C10—C19	117.53 (14)	O4—C26—H26C	109.5
C1^{i}—C10—C19	117.14 (14)	H26A—C26—H26C	109.5
C16—C11—C12	118.14 (15)	H26B—C26—H26C	109.5
C16—C11—C5	120.09 (15)	Cl2—C1S—Cl1	110.72 (12)
C12—C11—C5	121.74 (15)	Cl2—C1S—H1S1	109.5
O1—C12—C13	123.13 (16)	Cl1—C1S—H1S1	109.5
O1—C12—C11	115.86 (15)	Cl2—C1S—H1S2	109.5
C13—C12—C11	121.01 (16)	Cl1—C1S—H1S2	109.5
C14—C13—C12	119.10 (17)	H1S1—C1S—H1S2	108.1
C14—C13—H13	120.4	Cl4—C2S—Cl3	111.31 (11)
C12—C13—H13	120.4	Cl4—C2S—H2S1	109.4
C15—C14—C13	121.63 (17)	Cl3—C2S—H2S1	109.4
C15—C14—H14	119.2	Cl4—C2S—H2S2	109.4
C13—C14—H14	119.2	Cl3—C2S—H2S2	109.4
C14—C15—C16	118.99 (17)	H2S1—C2S—H2S2	108.0

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

Fig. 1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C12
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C17
C13