Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2,5-Bis[4-methyl-3-(pyridin-3-yl)-phenyl]-1,3,4-oxadiazole and its one-dimensional polymeric complex with $ZnCl_2$

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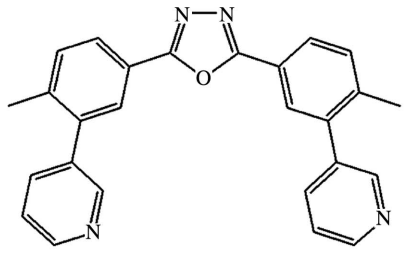
Received 22 December 2012
Accepted 7 August 2013

2,5-Bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole (*L*), $C_{26}H_{20}N_4O$, forms one-dimensional chains *via* two types of intermolecular π–π interactions. In *catena*-poly[[dichloridozinc(II)]-μ-2,5-bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole], $[ZnCl_2(C_{26}H_{20}N_4O)]_n$, synthesized by the combination of *L* with $ZnCl_2$, the Zn^{II} centres are coordinated by two Cl atoms and two N atoms from two *L* ligands. $[ZnCl_2L]_n$ forms one-dimensional *P* (plus) and *M* (minus) helical chains, where the *L* ligand has different directions of twist. The helical chains stack together *via* interchain π–π and C—H$\cdots\pi$ interactions.

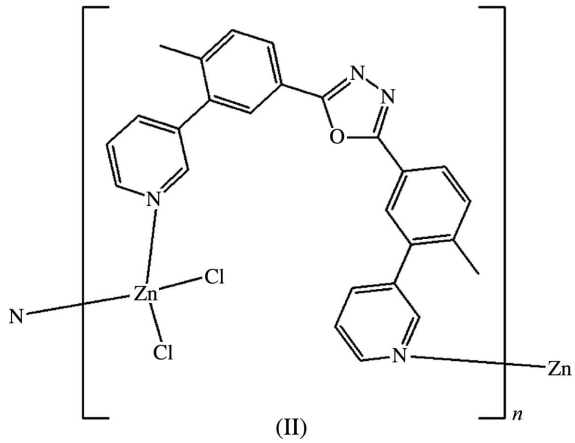
Keywords: crystal structure; MOFs; coordination polymers; helical chains.

1. Introduction

Numerous coordination polymers designed and constructed through crystal engineering have attracted significant attention because of their fascinating structural topologies (Chakrabary *et al.*, 2011) and functional applications (Amouri *et al.*, 2012; Das *et al.*, 2012). It is well known that the selection of appropriate ligands as building blocks is a key point in the design and synthesis of functional coordination polymers. Over the past decade, the design and construction of rigid and flexible organic ligands bridged by 1,3,4-oxadiazole have been pursued due to the diversity of these ligands in coordination chemistry and their applications in functional materials (Jabbour *et al.*, 2002; Hughes & Bryce, 2005; Du *et al.*, 2010). It is well known that π–π and C—H$\cdots\pi$ interactions play an important role in determining the arrangement of coordination polymers incorporating these ligands (Das *et al.*, 2010; Gathergood *et al.*, 2003). In order to investigate how organic ligands bridged by 1,3,4-oxadiazole affect the arrangement of molecular complexes in self-assembled aggregates, we synthesized a new 1,3,4-oxadiazole bridging ligand, namely 2,5-bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole (*L*), (I). The combination of *L* with $ZnCl_2$ afforded $[ZnCl_2L]_n$, (II), which is a coordination polymer with one-dimensional chains linked by π–π and C—H$\cdots\pi$ interactions.



(I)



(II)

2. Experimental

2.1. Synthesis and crystallization

For the preparation of (I), a mixture of 2,5-bis(3-bromo-4-methylphenyl)-1,3,4-oxadiazole (4.08 g, 10.00 mmol), (pyridin-3-yl)boronic acid (2.71 g, 22.0 mmol), K_2CO_3 (4.15 g, 30.0 mmol), $Pd(PPh_3)_4$ (1.16 g, 1.00 mmol) in an EtOH–H_2O (2:1 *v*/*v*) system were stirred under N_2 for 36 h under reflux. After removal of the solvent under vacuum, the residue was purified by silica-gel column chromatography using tetrahydrofuran (THF) and dichloromethane (DCM) (3:1 *v*/*v*) as eluent to afford (I) (yield 3.23 g, 80.3%). A solution of (I) (8.1 mg, 0.010 mmol) in CH_2Cl_2 (10 ml) was left for about 2 d at room temperature, after which time colourless crystals were obtained (yield 5.3 mg, 65.1%). IR (KBr pellet cm^{-1}): 3041 (*w*), 1616 (*ms*), 1589 (*s*), 1499 (*s*), 1385 (*vs*), 1238 (*s*), 1073 (*ms*), 898 (*ms*), 810 (*s*), 734 (*vs*), 719 (*s*). ^1H NMR (300 MHz, $CDCl_3$, 298 K, TMS): δ 8.64–8.65 (*t*, 2H, $-C_5H_4N$), 8.08–8.210 (*d*, 1H, –benzeneH_3), 7.98 (*s*, 1H, –benzeneH_3), 7.72–7.74 (*d*, 1H, –benzeneH_3), 7.46–7.49 (*d*, 1H, $-C_5H_4N$), 7.42–7.45 (*t*, 1H, –benzeneH_3), 2.36 (*s*, 3H, $-CH_3$). Elemental analysis (%) calculated for $C_{26}H_{20}N_4O$: C 77.21, H 4.98, N 13.85; found: C 77.42, H 4.82, N 13.85.

For the preparation of (II), a solution of $ZnCl_2$ (1.4 mg, 0.01 mmol) in MeOH (1 ml) was layered onto a solution of *L* (4.0 mg, 0.01 mmol) in tetrahydrofuran (2 ml). The solutions

  doi:10.1107/S0108270113022105

Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{26}H_{20}N_4O$	$[ZnCl_2(C_{26}H_{20}N_4O)]$
M_r	404.46	540.73
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	298	173
a, b, c (Å)	12.786 (3), 7.8720 (18), 20.732 (5)	17.779 (3), 7.3406 (14), 18.944 (4)
β (°)	105.573 (3)	102.942 (2)
V (Å^3)	2010.2 (8)	2409.6 (8)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.08	1.27
Crystal size (mm)	0.50 × 0.50 × 0.13	0.40 × 0.25 × 0.02
Data collection		
Diffractometer	Bruker SMART CCD area-detector diffractometer	Bruker SMART CCD area-detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)	Multi-scan (*SADABS*; Bruker, 2003)
T_{min}, T_{max}	0.959, 0.989	0.596, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10264, 3790, 3079	12117, 4524, 3375
R_{int}	0.023	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.608	0.608
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.122, 1.03	0.043, 0.111, 1.01
No. of reflections	3790	4522
No. of parameters	282	309
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.23	0.45, −0.36

Computer programs: *SMART* (Bruker, 2003), *SAINT* (Bruker, 2003), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) and *SHELXTL* (Sheldrick, 2008).

were left for about 6 d at room temperature after which time colourless crystals of (II) were obtained (yield 3.4 mg, 63%). IR (KBr pellet cm^{-1}): 2974 (*w*), 1616 (*ms*), 1550 (*s*), 1495 (*vs*), 1417 (*vs*), 1195 (*s*), 1036 (*ms*), 900 (*s*), 815 (*s*), 735 (*s*), 712(*vs*). Elemental analysis (%) calculated for $C_{26}H_{20}Cl_2N_4OZn$: C 57.75, H 3.73, N 10.36; found: C 57.83, H 3.74, N 10.37.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms attached to anisotropically refined atoms were placed in geometrically idealized positions and included as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms. The initial torsion angles of the methyl groups were established using a local difference Fourier calculation. In the refinement, the methyl groups were allowed to rotate.

3. Results and discussion

Within 2,5-bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole, (I) (Fig. 1), the dihedral angles between the planes of the pyridine and oxadiazole rings are 60.661 (6) and

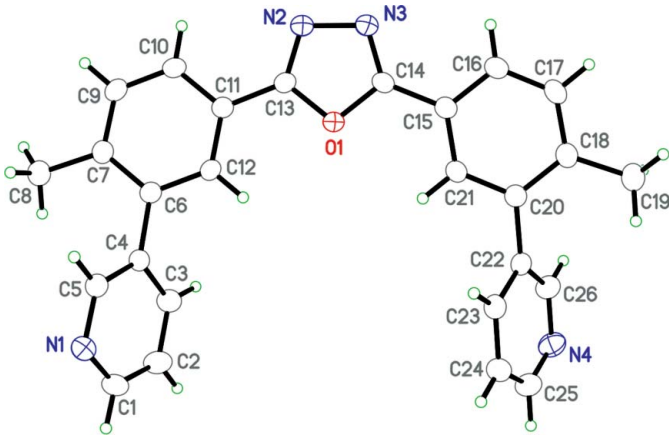


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

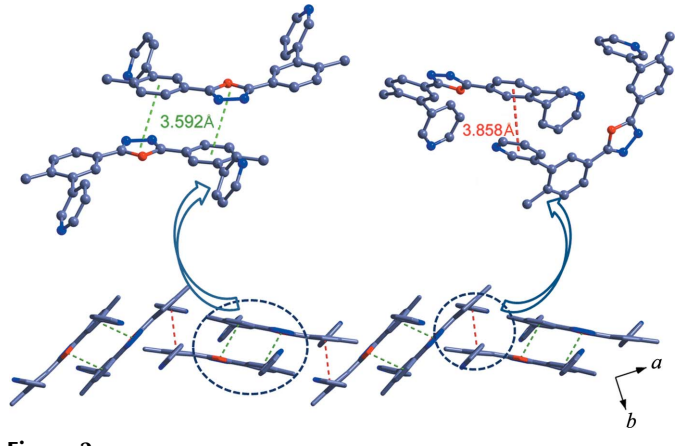


Figure 2
The one-dimensional chain of (I), constructed by two kinds of π–π interactions (red and green dashed lines in the electronic version of the paper). H atoms have been omitted for clarity.

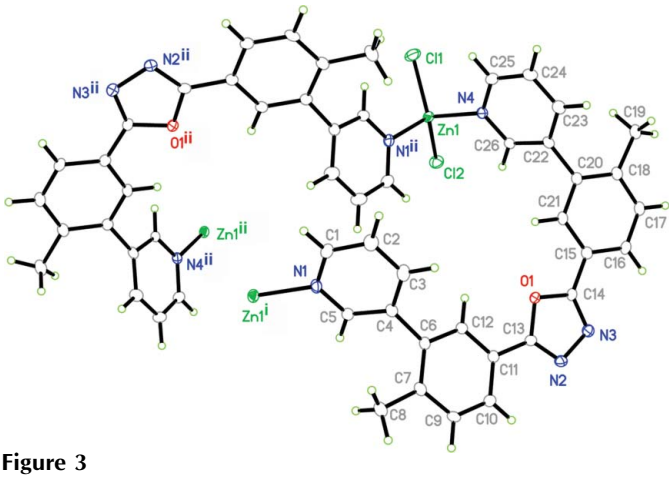


Figure 3
The molecular structure of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.]

58.169 (6)° for the N1- and N4-containing pyridine rings, respectively, and the dihedral angles between the pyridine rings and the adjacent benzene rings are 60.973 (5) and 51.894 (4)°. The two benzene rings of (I) are almost coplanar, with a dihedral angle of 8.977 (4)° between the planes.

Molecules of (I) are arranged in chains *via* two kinds of π–π interactions (Fig. 2). One type is between the oxadiazole ring of one molecule and a benzene ring of an adjacent molecule [centroid–centroid distance = 3.592 (1) Å], while the other is between a benzene ring of one molecule and the N4-containing pyridine ring of a neighbouring molecule [centroid–centroid distance = 3.858 (3) Å].

Compound (II) crystallizes with one Zn^{II} centre in a distorted tetrahedral environment ($ZnCl_2N_2$) involving two Cl atoms (Cl1 and Cl2) and two N atoms from two *L* ligands [N1^{ii} and N4; symmetry code: (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$] (Fig. 3). The coordination behaviour of the Zn^{II} atom is similar to that of the Hg^{II} atom in Hg{2,5-bis(pyridin-3-yl)-1,3,4-oxadiazole}I_2 (Dong *et al.*, 2003), which is coordinated by two N-atom donors from two oxadiazole bridging ligands and two coordinated iodide ligands.

Compared with the dihedral angles given above for (I), those in (II) between the pyridine rings and the adjacent benzene rings change to 53.464 (1) and 56.966 (1)° for the N1- and N4-containing pyridine rings, respectively. Additionally, the dihedral angle formed by the two benzene rings changes from 8.977 (4)° in the free ligand to 11.887 (9)° in (II). In the extended structure of (II), complex molecules are joined to form a one-dimensional chain along the *b* axis (Fig. 4). It is interesting that *L* has different directions of twist when coordinated to the Zn^{II} centre. It is also the origin of the presence of *P* (plus) and *M* (minus) helices in (II). To our knowledge, reports of such an arrangement of helical chains are rare in Zn^{II} frameworks (Yashima *et al.*, 2008; Bishop, 2008). It is similar to that found in $[Zn(mspda)(C_2H_7N)]_n$ [mspda^{2-} is (*E*)-2,6-dimethyl-4-styrylpyridine-3,5-dicarboxylate; Zhang *et al.*, 2012], which has two *S*- and *R*-type chiral units from the axially prochiral mspda^{2-}. These chiral units

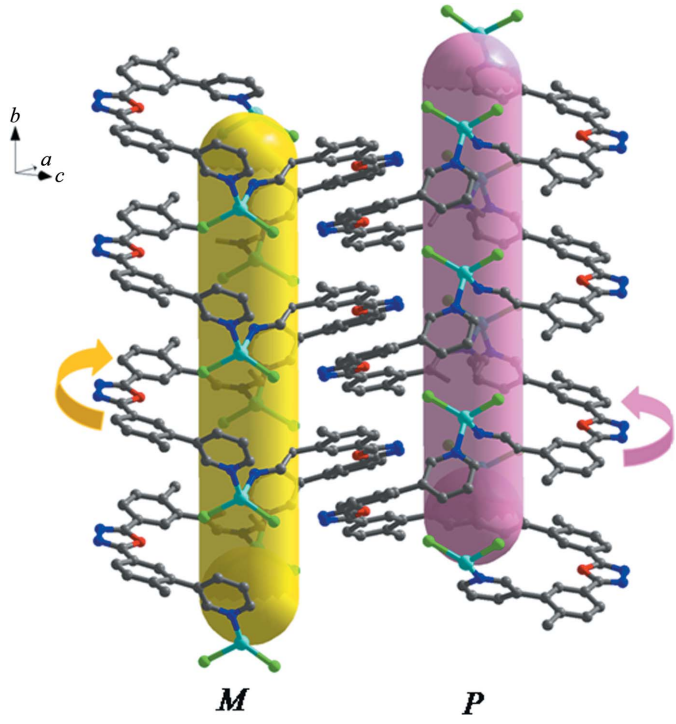


Figure 4
View of the one-dimensional *P* (plus) and *M* (minus) helices of (II), which are assembled by different ligand twists and Zn^{II} ions. H atoms have been omitted for clarity.

combined with Zn^{II} ions to assemble right-handed (*P*) and left-handed (*M*) Zn–mspda helical chains. Finally, the *P*- and *M*-type helical chains are interlinked by carboxylate O atoms to form a one-dimensional ladder.

The helical chains in (II) are arranged side-by-side along the *b* axis (Fig. 5), where they interact *via* two kinds of π–π interactions [centroid–centroid distances = 3.823 (1) and 3.556 (1) Å]. The result is that a novel two-dimensional sheet is generated in the *bc* plane. It is similar to that observed in a previously reported compound (Yang *et al.*, 2011), which forms helical chains that aggregate *via* interchain π–π interactions to extend the dimensionality of the structure from one- to two-dimensional. In (II), the two-dimensional sheets then interact *via* C—H$\cdots\pi$ interactions [H$\cdots$centroid distance = 2.755 (6) Å] along the *b* axis to form a novel coordination polymer. The distance is similar to that observed in morphine bis(1-naphthoate) (Gathergood *et al.*, 2003), where the H$\cdots$centroid distances are in the range 2.80–3.07 Å.

In summary, a new compound with *P*- and *M*-type helical chains has been successfully obtained based on the new flexible 1,3,4-oxadiazole-centred bridging ligand *L* and $ZnCl_2$. The helices assemble through interchain π–π and C—H$\cdots\pi$ interactions to form a novel coordination polymer. This study demonstrates that π–π and C—H$\cdots\pi$ interactions play an important role in constructing coordination polymers.

This work was supported by the National Natural Science Foundation of China (grant No. 21101100), the Shandong Distinguished Middle-Aged and Young Scientist Encourage

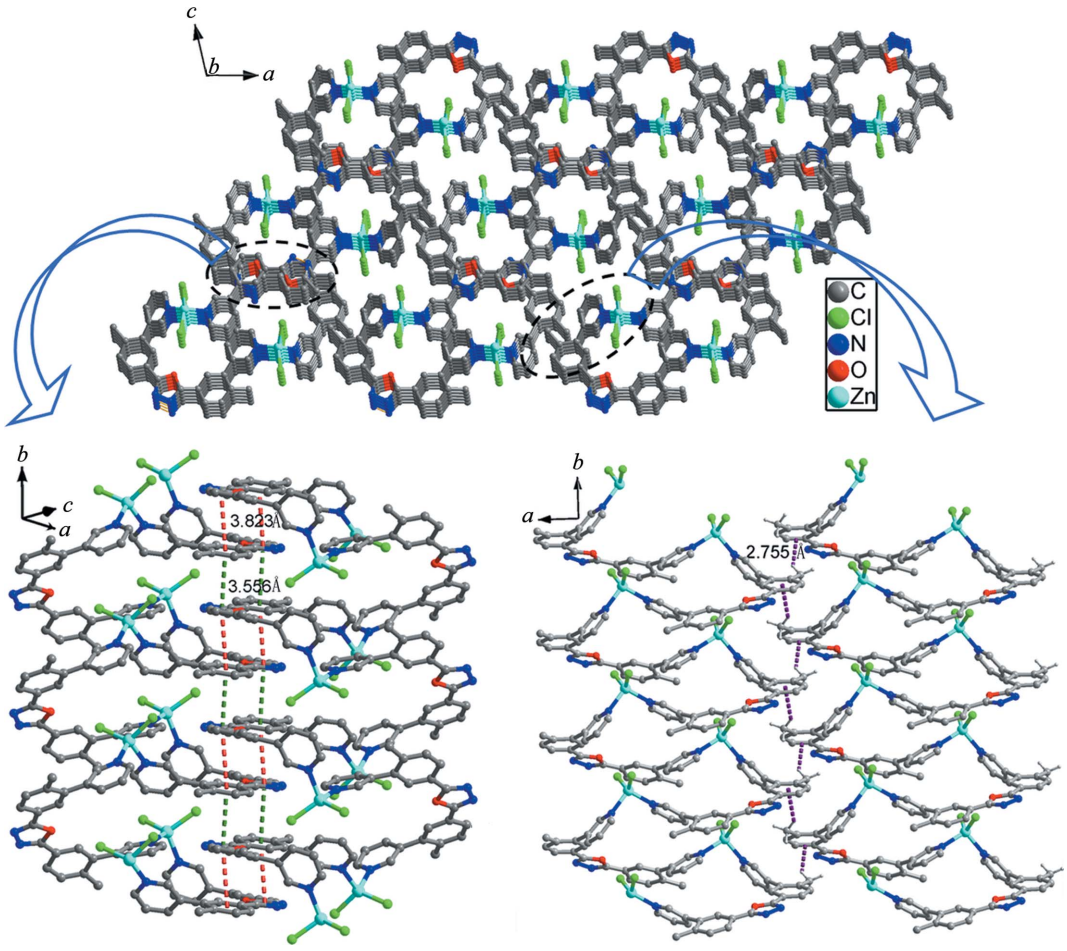


Figure 5
A packing view of (II), constructed by interchain π–π interactions (red and green dashed lines in the electronic version of the paper) and C—H$\cdots\pi$ interactions (purple dashed lines in the electronic version of the paper). Some H atoms have been omitted.

and Reward Foundation (grant No. BS2012CL035), 'PCSIRT' and Taishan scholars' construction project special fund.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: EM3058). Services for accessing these data are described at the back of the journal.

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supplementary materials

Acta Cryst. (2013). C**69**, 1108-1111 [doi:10.1107/S0108270113022105]

2,5-Bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole and its one-dimensional polymeric complex with $ZnCl_2$

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Computing details

For both compounds, data collection: *SMART* (Bruker, 2003); cell refinement: *SMART* (Bruker, 2003); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

(I) 2,5-Bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole

Crystal data

$C_{26}H_{20}N_4O$
M_r = 404.46
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
a = 12.786 (3) Å
b = 7.8720 (18) Å
c = 20.732 (5) Å
β = 105.573 (3)°
V = 2010.2 (8) Å^3
Z = 4
$F(000)$ = 848
D_x = 1.336 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4084 reflections
θ = 2.6–27.8°
μ = 0.08 mm^{-1}
T = 298 K
Block, colourless
0.50 × 0.50 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.959, T_{max} = 0.989
10264 measured reflections
3790 independent reflections
3079 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.6°, θ_{min} = 2.0°
h = −9→15
k = −9→9
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.03
3790 reflections
282 parameters
0 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

$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 0.4318P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.12513 (15)	0.2667 (3)	0.29172 (9)	0.0602 (5)
H1	−0.1429	0.2709	0.3323	0.072*
C2	−0.03144 (16)	0.1856 (3)	0.28994 (8)	0.0598 (5)
H2	0.0145	0.1398	0.3286	0.072*
C3	−0.00664 (14)	0.1734 (2)	0.22925 (8)	0.0508 (4)
H3	0.0562	0.1179	0.2265	0.061*
C4	−0.07560 (12)	0.2439 (2)	0.17264 (7)	0.0403 (4)
C5	−0.16687 (13)	0.3273 (2)	0.18080 (8)	0.0484 (4)
H5	−0.2132	0.3774	0.1432	0.058*
C6	−0.05221 (12)	0.23559 (19)	0.10603 (7)	0.0384 (3)
C7	−0.12393 (12)	0.1567 (2)	0.05105 (8)	0.0417 (4)
C8	−0.22349 (15)	0.0623 (2)	0.05632 (9)	0.0575 (5)
H8A	−0.2846	0.1380	0.0463	0.086*
H8B	−0.2121	0.0188	0.1009	0.086*
H8C	−0.2374	−0.0303	0.0250	0.086*
C9	−0.09938 (13)	0.1609 (2)	−0.01032 (8)	0.0448 (4)
H9	−0.1467	0.1101	−0.0473	0.054*
C10	−0.00730 (13)	0.2381 (2)	−0.01780 (7)	0.0436 (4)
H10	0.0066	0.2404	−0.0596	0.052*
C11	0.06540 (12)	0.31288 (18)	0.03691 (7)	0.0373 (3)
C12	0.04249 (12)	0.31020 (19)	0.09854 (7)	0.0383 (3)
H12	0.0911	0.3590	0.1355	0.046*
C13	0.16280 (11)	0.39487 (19)	0.02775 (7)	0.0373 (3)
C14	0.31299 (12)	0.52824 (19)	0.05390 (7)	0.0381 (3)
C15	0.40979 (12)	0.60686 (19)	0.09681 (7)	0.0390 (3)
C16	0.49126 (13)	0.6629 (2)	0.06909 (8)	0.0484 (4)
H16	0.4819	0.6567	0.0231	0.058*
C17	0.58554 (14)	0.7274 (2)	0.10996 (8)	0.0518 (4)
H17	0.6388	0.7663	0.0906	0.062*
C18	0.60463 (12)	0.7369 (2)	0.17899 (8)	0.0446 (4)
C19	0.70939 (14)	0.8139 (3)	0.21953 (9)	0.0619 (5)
H19A	0.7680	0.7365	0.2210	0.093*
H19B	0.7046	0.8357	0.2642	0.093*

H19C	0.7224	0.9186	0.1992	0.093*
C20	0.52395 (12)	0.67559 (19)	0.20748 (7)	0.0387 (4)
C21	0.42699 (12)	0.61574 (19)	0.16563 (7)	0.0381 (3)
H21	0.3721	0.5807	0.1844	0.046*
C22	0.53833 (12)	0.66639 (19)	0.28099 (7)	0.0392 (4)
C23	0.46033 (12)	0.7284 (2)	0.30991 (8)	0.0441 (4)
H23	0.3986	0.7819	0.2837	0.053*
C24	0.47466 (14)	0.7104 (2)	0.37778 (8)	0.0525 (4)
H24	0.4229	0.7511	0.3980	0.063*
C25	0.56682 (16)	0.6311 (2)	0.41499 (9)	0.0572 (5)
H25	0.5761	0.6202	0.4608	0.069*
C26	0.62796 (13)	0.5867 (2)	0.32332 (8)	0.0493 (4)
H26	0.6804	0.5428	0.3044	0.059*
N1	−0.19268 (12)	0.3404 (2)	0.23861 (7)	0.0577 (4)
N2	0.19136 (11)	0.41233 (18)	−0.02684 (6)	0.0460 (3)
N3	0.29032 (11)	0.50044 (18)	−0.00966 (6)	0.0464 (3)
N4	0.64377 (12)	0.5689 (2)	0.38922 (7)	0.0582 (4)
O1	0.23554 (8)	0.46532 (13)	0.08148 (5)	0.0388 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0610 (11)	0.0840 (14)	0.0404 (9)	−0.0090 (10)	0.0216 (8)	−0.0022 (9)
C2	0.0670 (12)	0.0720 (13)	0.0387 (9)	0.0045 (10)	0.0114 (8)	0.0102 (8)
C3	0.0478 (9)	0.0608 (11)	0.0433 (9)	0.0059 (8)	0.0116 (7)	0.0043 (8)
C4	0.0383 (8)	0.0452 (9)	0.0375 (8)	−0.0086 (7)	0.0102 (6)	−0.0018 (6)
C5	0.0382 (8)	0.0658 (11)	0.0400 (8)	−0.0018 (8)	0.0087 (7)	−0.0026 (8)
C6	0.0377 (8)	0.0412 (8)	0.0356 (8)	0.0008 (6)	0.0089 (6)	0.0001 (6)
C7	0.0401 (8)	0.0406 (8)	0.0433 (8)	−0.0038 (7)	0.0093 (7)	−0.0019 (7)
C8	0.0539 (10)	0.0656 (12)	0.0533 (10)	−0.0209 (9)	0.0149 (8)	−0.0101 (9)
C9	0.0455 (9)	0.0482 (9)	0.0369 (8)	−0.0063 (7)	0.0044 (7)	−0.0062 (7)
C10	0.0476 (9)	0.0504 (9)	0.0321 (8)	−0.0021 (7)	0.0095 (7)	−0.0013 (7)
C11	0.0373 (8)	0.0391 (8)	0.0354 (8)	0.0023 (6)	0.0095 (6)	0.0009 (6)
C12	0.0351 (7)	0.0445 (8)	0.0330 (7)	−0.0010 (6)	0.0053 (6)	−0.0035 (6)
C13	0.0373 (8)	0.0414 (8)	0.0321 (7)	0.0020 (6)	0.0073 (6)	−0.0018 (6)
C14	0.0372 (8)	0.0431 (8)	0.0365 (8)	0.0021 (6)	0.0142 (6)	0.0040 (6)
C15	0.0383 (8)	0.0409 (8)	0.0388 (8)	0.0016 (7)	0.0117 (6)	0.0044 (6)
C16	0.0501 (9)	0.0582 (10)	0.0403 (8)	−0.0061 (8)	0.0177 (7)	0.0018 (7)
C17	0.0458 (9)	0.0631 (11)	0.0525 (10)	−0.0113 (8)	0.0236 (8)	−0.0003 (8)
C18	0.0375 (8)	0.0478 (9)	0.0499 (9)	−0.0015 (7)	0.0139 (7)	−0.0012 (7)
C19	0.0436 (10)	0.0804 (14)	0.0624 (11)	−0.0131 (9)	0.0154 (8)	−0.0065 (10)
C20	0.0367 (8)	0.0392 (8)	0.0404 (8)	0.0026 (6)	0.0105 (6)	0.0015 (6)
C21	0.0343 (7)	0.0426 (8)	0.0388 (8)	0.0004 (6)	0.0124 (6)	0.0034 (6)
C22	0.0377 (8)	0.0388 (8)	0.0398 (8)	−0.0038 (6)	0.0080 (6)	−0.0015 (6)
C23	0.0378 (8)	0.0481 (9)	0.0451 (9)	−0.0019 (7)	0.0087 (7)	0.0016 (7)
C24	0.0512 (10)	0.0627 (11)	0.0468 (9)	−0.0048 (8)	0.0186 (8)	−0.0038 (8)
C25	0.0628 (11)	0.0675 (12)	0.0387 (9)	−0.0038 (10)	0.0090 (8)	0.0021 (8)
C26	0.0447 (9)	0.0556 (10)	0.0450 (9)	0.0055 (8)	0.0075 (7)	−0.0022 (8)
N1	0.0441 (8)	0.0849 (11)	0.0468 (8)	−0.0035 (8)	0.0167 (7)	−0.0084 (8)
N2	0.0450 (7)	0.0596 (8)	0.0350 (7)	−0.0059 (7)	0.0131 (6)	−0.0037 (6)

N3	0.0428 (7)	0.0618 (9)	0.0364 (7)	−0.0051 (6)	0.0141 (6)	−0.0022 (6)
N4	0.0580 (9)	0.0657 (10)	0.0440 (8)	0.0060 (8)	0.0019 (7)	0.0035 (7)
O1	0.0376 (5)	0.0476 (6)	0.0317 (5)	−0.0034 (5)	0.0101 (4)	−0.0001 (4)

Geometric parameters (Å, º)

C1—N1	1.336 (2)	C14—O1	1.3627 (17)
C1—C2	1.367 (3)	C14—C15	1.454 (2)
C1—H1	0.9300	C15—C21	1.386 (2)
C2—C3	1.381 (2)	C15—C16	1.390 (2)
C2—H2	0.9300	C16—C17	1.371 (2)
C3—C4	1.381 (2)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.388 (2)
C4—C5	1.388 (2)	C17—H17	0.9300
C4—C6	1.491 (2)	C18—C20	1.405 (2)
C5—N1	1.330 (2)	C18—C19	1.504 (2)
C5—H5	0.9300	C19—H19A	0.9600
C6—C12	1.391 (2)	C19—H19B	0.9600
C6—C7	1.402 (2)	C19—H19C	0.9600
C7—C9	1.390 (2)	C20—C21	1.391 (2)
C7—C8	1.503 (2)	C20—C22	1.487 (2)
C8—H8A	0.9600	C21—H21	0.9300
C8—H8B	0.9600	C22—C23	1.383 (2)
C8—H8C	0.9600	C22—C26	1.392 (2)
C9—C10	1.370 (2)	C23—C24	1.377 (2)
C9—H9	0.9300	C23—H23	0.9300
C10—C11	1.390 (2)	C24—C25	1.373 (3)
C10—H10	0.9300	C24—H24	0.9300
C11—C12	1.385 (2)	C25—N4	1.332 (2)
C11—C13	1.460 (2)	C25—H25	0.9300
C12—H12	0.9300	C26—N4	1.334 (2)
C13—N2	1.2867 (19)	C26—H26	0.9300
C13—O1	1.3627 (17)	N2—N3	1.4025 (19)
C14—N3	1.2896 (19)		

N1—C1—C2	123.92 (16)	C21—C15—C16	118.70 (14)
N1—C1—H1	118.0	C21—C15—C14	121.67 (13)
C2—C1—H1	118.0	C16—C15—C14	119.44 (14)
C1—C2—C3	118.33 (16)	C17—C16—C15	119.62 (15)
C1—C2—H2	120.8	C17—C16—H16	120.2
C3—C2—H2	120.8	C15—C16—H16	120.2
C4—C3—C2	119.71 (16)	C16—C17—C18	122.63 (15)
C4—C3—H3	120.1	C16—C17—H17	118.7
C2—C3—H3	120.1	C18—C17—H17	118.7
C3—C4—C5	116.90 (14)	C17—C18—C20	117.99 (14)
C3—C4—C6	121.90 (14)	C17—C18—C19	118.80 (14)
C5—C4—C6	121.19 (14)	C20—C18—C19	123.21 (15)
N1—C5—C4	124.52 (16)	C18—C19—H19A	109.5
N1—C5—H5	117.7	C18—C19—H19B	109.5
C4—C5—H5	117.7	H19A—C19—H19B	109.5

C12—C6—C7	119.68 (13)	C18—C19—H19C	109.5
C12—C6—C4	118.81 (13)	H19A—C19—H19C	109.5
C7—C6—C4	121.51 (13)	H19B—C19—H19C	109.5
C9—C7—C6	118.33 (14)	C21—C20—C18	119.10 (14)
C9—C7—C8	118.81 (14)	C21—C20—C22	117.85 (13)
C6—C7—C8	122.82 (14)	C18—C20—C22	123.02 (13)
C7—C8—H8A	109.5	C15—C21—C20	121.87 (14)
C7—C8—H8B	109.5	C15—C21—H21	119.1
H8A—C8—H8B	109.5	C20—C21—H21	119.1
C7—C8—H8C	109.5	C23—C22—C26	116.95 (14)
H8A—C8—H8C	109.5	C23—C22—C20	121.45 (13)
H8B—C8—H8C	109.5	C26—C22—C20	121.50 (14)
C10—C9—C7	121.76 (14)	C24—C23—C22	119.54 (15)
C10—C9—H9	119.1	C24—C23—H23	120.2
C7—C9—H9	119.1	C22—C23—H23	120.2
C9—C10—C11	120.14 (14)	C25—C24—C23	118.67 (16)
C9—C10—H10	119.9	C25—C24—H24	120.7
C11—C10—H10	119.9	C23—C24—H24	120.7
C12—C11—C10	119.05 (14)	N4—C25—C24	123.82 (16)
C12—C11—C13	121.72 (13)	N4—C25—H25	118.1
C10—C11—C13	119.23 (13)	C24—C25—H25	118.1
C11—C12—C6	121.01 (13)	N4—C26—C22	124.47 (16)
C11—C12—H12	119.5	N4—C26—H26	117.8
C6—C12—H12	119.5	C22—C26—H26	117.8
N2—C13—O1	112.51 (13)	C5—N1—C1	116.57 (15)
N2—C13—C11	127.97 (13)	C13—N2—N3	106.21 (12)
O1—C13—C11	119.51 (12)	C14—N3—N2	106.47 (12)
N3—C14—O1	112.19 (13)	C25—N4—C26	116.55 (15)
N3—C14—C15	128.18 (13)	C14—O1—C13	102.62 (11)
O1—C14—C15	119.54 (12)		

(II) *catena*-Poly[[dichloridozinc(II)]-μ-2,5-bis[4-methyl-3-(pyridin-3-yl)phenyl]-1,3,4-oxadiazole]

Crystal data

$ZnCl_2(C_{26}H_{20}N_4O)]$
M_r = 540.73
Monoclinic, $P2_1/n$
Hall symbol: -P2yn
a = 17.779 (3) Å
b = 7.3406 (14) Å
c = 18.944 (4) Å
β = 102.942 (2)°
V = 2409.6 (8) Å^3
Z = 4
$F(000)$ = 1104
D_x = 1.491 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2427 reflections
θ = 2.4–24.2°
μ = 1.27 mm^{-1}
T = 173 K
Plan, colourless
0.40 × 0.25 × 0.02 mm

Data collection

CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.596, T_{max} = 0.975
12117 measured reflections
4524 independent reflections
3375 reflections with $I > 2\sigma(I)$

R_{int} = 0.047
θ_{max} = 25.6°, θ_{min} = 1.4°
h = −20→21
k = −8→7
l = −18→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.01
4522 reflections
309 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.1756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.16126 (18)	0.6976 (5)	0.26063 (18)	0.0328 (8)
H1	0.1209	0.6833	0.2187	0.039*
C2	0.2280 (2)	0.7857 (6)	0.25466 (19)	0.0431 (10)
H2	0.2347	0.8265	0.2089	0.052*
C3	0.2849 (2)	0.8137 (5)	0.31622 (19)	0.0390 (9)
H3	0.3313	0.8736	0.3129	0.047*
C4	0.27476 (16)	0.7550 (4)	0.38297 (16)	0.0247 (7)
C5	0.20737 (16)	0.6597 (4)	0.38309 (16)	0.0246 (7)
H5	0.2005	0.6118	0.4278	0.030*
C6	0.33366 (17)	0.7906 (4)	0.45015 (16)	0.0223 (7)
C7	0.31546 (17)	0.8769 (4)	0.51069 (17)	0.0246 (7)
C8	0.23458 (18)	0.9378 (5)	0.51220 (19)	0.0354 (9)
H8A	0.2046	0.8329	0.5223	0.053*
H8B	0.2099	0.9901	0.4651	0.053*
H8C	0.2369	1.0298	0.5501	0.053*
C9	0.37515 (18)	0.9106 (5)	0.57054 (17)	0.0274 (8)
H9	0.3636	0.9689	0.6116	0.033*
C10	0.45045 (17)	0.8624 (4)	0.57237 (16)	0.0250 (7)
H10	0.4899	0.8878	0.6140	0.030*
C11	0.46819 (17)	0.7764 (4)	0.51290 (16)	0.0223 (7)
C12	0.41013 (16)	0.7427 (4)	0.45214 (16)	0.0224 (7)
H12	0.4225	0.6860	0.4111	0.027*
C13	0.54849 (17)	0.7289 (4)	0.51408 (16)	0.0220 (7)

C14	0.64252 (16)	0.6395 (4)	0.47064 (16)	0.0214 (7)
C15	0.68035 (17)	0.5769 (4)	0.41447 (16)	0.0224 (7)
C16	0.76060 (17)	0.5720 (4)	0.42672 (17)	0.0249 (7)
H16	0.7914	0.6053	0.4726	0.030*
C17	0.79496 (18)	0.5185 (4)	0.37161 (18)	0.0274 (7)
H17	0.8497	0.5136	0.3808	0.033*
C18	0.75261 (18)	0.4716 (4)	0.30340 (17)	0.0249 (7)
C19	0.79327 (18)	0.4310 (5)	0.24346 (18)	0.0312 (8)
H19A	0.7984	0.5435	0.2171	0.047*
H19B	0.7632	0.3420	0.2101	0.047*
H19C	0.8446	0.3811	0.2642	0.047*
C20	0.67094 (17)	0.4712 (4)	0.29199 (16)	0.0217 (7)
C21	0.63684 (17)	0.5235 (4)	0.34775 (16)	0.0229 (7)
H21	0.5822	0.5227	0.3400	0.027*
C22	0.61998 (17)	0.4131 (4)	0.22197 (16)	0.0234 (7)
C23	0.6204 (2)	0.4928 (5)	0.15529 (18)	0.0316 (8)
H23	0.6543	0.5912	0.1525	0.038*
C24	0.57161 (19)	0.4284 (5)	0.09361 (18)	0.0337 (8)
H24	0.5717	0.4811	0.0478	0.040*
C25	0.52253 (18)	0.2863 (5)	0.09907 (17)	0.0309 (8)
H25	0.4895	0.2408	0.0562	0.037*
C26	0.56744 (16)	0.2750 (4)	0.22232 (16)	0.0226 (7)
H26	0.5649	0.2228	0.2676	0.027*
Cl1	0.43174 (5)	−0.15244 (14)	0.06523 (5)	0.0459 (3)
Cl2	0.49046 (5)	−0.14652 (13)	0.27360 (4)	0.0363 (2)
N1	0.15169 (13)	0.6314 (4)	0.32396 (14)	0.0257 (6)
N2	0.60893 (14)	0.7419 (4)	0.56605 (13)	0.0275 (6)
N3	0.67166 (14)	0.6846 (4)	0.53745 (14)	0.0268 (6)
N4	0.51988 (13)	0.2103 (4)	0.16266 (13)	0.0251 (6)
O1	0.56427 (11)	0.6635 (3)	0.45198 (10)	0.0220 (5)
Zn1	0.44697 (2)	−0.00636 (5)	0.169115 (19)	0.02624 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0243 (17)	0.045 (2)	0.0259 (18)	−0.0039 (16)	−0.0009 (14)	0.0018 (16)
C2	0.038 (2)	0.061 (3)	0.029 (2)	−0.0107 (19)	0.0046 (17)	0.0120 (18)
C3	0.0313 (19)	0.050 (3)	0.034 (2)	−0.0132 (18)	0.0043 (16)	0.0080 (18)
C4	0.0213 (16)	0.0289 (19)	0.0244 (17)	0.0017 (14)	0.0058 (13)	0.0024 (14)
C5	0.0236 (16)	0.0288 (19)	0.0217 (17)	−0.0021 (14)	0.0056 (14)	0.0013 (14)
C6	0.0232 (16)	0.0222 (18)	0.0221 (17)	−0.0058 (13)	0.0062 (13)	0.0031 (13)
C7	0.0261 (16)	0.0207 (18)	0.0295 (18)	−0.0020 (14)	0.0116 (14)	0.0044 (14)
C8	0.0284 (18)	0.040 (2)	0.042 (2)	−0.0009 (16)	0.0151 (17)	−0.0053 (17)
C9	0.0341 (19)	0.0291 (19)	0.0232 (18)	−0.0057 (16)	0.0156 (15)	−0.0050 (14)
C10	0.0275 (17)	0.0269 (19)	0.0203 (17)	−0.0041 (14)	0.0048 (14)	0.0015 (14)
C11	0.0243 (16)	0.0219 (17)	0.0216 (17)	−0.0041 (13)	0.0067 (14)	0.0024 (13)
C12	0.0238 (16)	0.0232 (18)	0.0210 (16)	−0.0025 (13)	0.0064 (13)	0.0014 (13)
C13	0.0265 (17)	0.0223 (18)	0.0175 (16)	−0.0027 (14)	0.0058 (14)	0.0012 (13)
C14	0.0181 (15)	0.0218 (17)	0.0229 (17)	−0.0015 (13)	0.0011 (13)	0.0027 (13)
C15	0.0220 (16)	0.0205 (17)	0.0242 (17)	0.0012 (14)	0.0040 (13)	0.0041 (13)

C16	0.0215 (16)	0.0231 (18)	0.0267 (18)	−0.0029 (14)	−0.0017 (14)	0.0055 (14)
C17	0.0194 (16)	0.0277 (19)	0.0350 (19)	−0.0014 (14)	0.0061 (14)	0.0001 (15)
C18	0.0232 (16)	0.0200 (18)	0.0326 (19)	0.0003 (13)	0.0085 (14)	0.0014 (14)
C19	0.0256 (17)	0.0270 (19)	0.043 (2)	−0.0021 (15)	0.0125 (16)	−0.0061 (16)
C20	0.0221 (16)	0.0178 (17)	0.0251 (17)	−0.0001 (13)	0.0051 (13)	0.0026 (13)
C21	0.0176 (15)	0.0211 (18)	0.0293 (18)	−0.0001 (13)	0.0040 (13)	0.0041 (14)
C22	0.0204 (16)	0.0261 (18)	0.0261 (18)	0.0043 (14)	0.0102 (13)	0.0003 (14)
C23	0.0331 (19)	0.031 (2)	0.032 (2)	−0.0017 (16)	0.0101 (16)	0.0019 (16)
C24	0.0354 (19)	0.044 (2)	0.0216 (18)	0.0021 (17)	0.0070 (15)	0.0052 (16)
C25	0.0260 (17)	0.043 (2)	0.0217 (18)	−0.0004 (16)	0.0015 (14)	−0.0003 (15)
C26	0.0167 (15)	0.0308 (19)	0.0204 (17)	0.0026 (14)	0.0044 (13)	0.0002 (14)
Cl1	0.0396 (5)	0.0636 (7)	0.0312 (5)	0.0066 (5)	0.0008 (4)	−0.0189 (5)
Cl2	0.0360 (5)	0.0419 (6)	0.0283 (5)	0.0047 (4)	0.0015 (4)	0.0037 (4)
N1	0.0177 (13)	0.0319 (17)	0.0269 (15)	0.0001 (12)	0.0037 (11)	0.0035 (12)
N2	0.0255 (14)	0.0376 (18)	0.0190 (14)	0.0001 (13)	0.0046 (12)	−0.0013 (12)
N3	0.0226 (14)	0.0332 (17)	0.0237 (15)	−0.0003 (12)	0.0032 (12)	0.0009 (12)
N4	0.0187 (13)	0.0341 (17)	0.0223 (15)	0.0012 (12)	0.0045 (11)	−0.0012 (12)
O1	0.0183 (10)	0.0271 (13)	0.0196 (11)	−0.0010 (9)	0.0020 (9)	−0.0011 (9)
Zn1	0.0189 (2)	0.0357 (3)	0.0227 (2)	0.00116 (17)	0.00174 (15)	−0.00337 (17)

Geometric parameters (Å, º)

C1—N1	1.340 (4)	C15—C21	1.383 (4)
C1—C2	1.378 (5)	C15—C16	1.394 (4)
C1—H1	0.9500	C16—C17	1.380 (4)
C2—C3	1.377 (5)	C16—H16	0.9500
C2—H2	0.9500	C17—C18	1.385 (4)
C3—C4	1.385 (4)	C17—H17	0.9500
C3—H3	0.9500	C18—C20	1.419 (4)
C4—C5	1.388 (4)	C18—C19	1.506 (4)
C4—C6	1.479 (4)	C19—H19A	0.9800
C5—N1	1.335 (4)	C19—H19B	0.9800
C5—H5	0.9500	C19—H19C	0.9800
C6—C12	1.397 (4)	C20—C21	1.385 (4)
C6—C7	1.410 (4)	C20—C22	1.491 (4)
C7—C9	1.391 (4)	C21—H21	0.9500
C7—C8	1.512 (4)	C22—C26	1.379 (4)
C8—H8A	0.9800	C22—C23	1.393 (4)
C8—H8B	0.9800	C23—C24	1.374 (5)
C8—H8C	0.9800	C23—H23	0.9500
C9—C10	1.377 (4)	C24—C25	1.379 (5)
C9—H9	0.9500	C24—H24	0.9500
C10—C11	1.388 (4)	C25—N4	1.338 (4)
C10—H10	0.9500	C25—H25	0.9500
C11—C12	1.386 (4)	C26—N4	1.338 (4)
C11—C13	1.465 (4)	C26—H26	0.9500
C12—H12	0.9500	Cl1—Zn1	2.2040 (10)
C13—N2	1.288 (4)	Cl2—Zn1	2.2111 (10)
C13—O1	1.357 (3)	N1—Zn1^{i}	2.054 (2)
C14—N3	1.298 (4)	N2—N3	1.409 (3)

C14—O1	1.368 (3)	N4—Zn1	2.073 (3)
C14—C15	1.455 (4)	Zn1—N1^{ii}	2.054 (2)
N1—C1—C2	121.9 (3)	C15—C16—H16	120.3
N1—C1—H1	119.1	C16—C17—C18	122.4 (3)
C2—C1—H1	119.1	C16—C17—H17	118.8
C3—C2—C1	118.9 (3)	C18—C17—H17	118.8
C3—C2—H2	120.6	C17—C18—C20	117.8 (3)
C1—C2—H2	120.6	C17—C18—C19	120.0 (3)
C2—C3—C4	120.4 (3)	C20—C18—C19	122.1 (3)
C2—C3—H3	119.8	C18—C19—H19A	109.5
C4—C3—H3	119.8	C18—C19—H19B	109.5
C3—C4—C5	116.6 (3)	H19A—C19—H19B	109.5
C3—C4—C6	121.2 (3)	C18—C19—H19C	109.5
C5—C4—C6	122.2 (3)	H19A—C19—H19C	109.5
N1—C5—C4	123.7 (3)	H19B—C19—H19C	109.5
N1—C5—H5	118.1	C21—C20—C18	119.4 (3)
C4—C5—H5	118.1	C21—C20—C22	118.4 (3)
C12—C6—C7	119.4 (3)	C18—C20—C22	122.2 (3)
C12—C6—C4	118.4 (3)	C15—C21—C20	121.7 (3)
C7—C6—C4	122.2 (3)	C15—C21—H21	119.2
C9—C7—C6	118.1 (3)	C20—C21—H21	119.2
C9—C7—C8	119.2 (3)	C26—C22—C23	117.0 (3)
C6—C7—C8	122.7 (3)	C26—C22—C20	118.9 (3)
C7—C8—H8A	109.5	C23—C22—C20	124.1 (3)
C7—C8—H8B	109.5	C24—C23—C22	119.8 (3)
H8A—C8—H8B	109.5	C24—C23—H23	120.1
C7—C8—H8C	109.5	C22—C23—H23	120.1
H8A—C8—H8C	109.5	C23—C24—C25	119.1 (3)
H8B—C8—H8C	109.5	C23—C24—H24	120.5
C10—C9—C7	122.3 (3)	C25—C24—H24	120.5
C10—C9—H9	118.8	N4—C25—C24	122.2 (3)
C7—C9—H9	118.8	N4—C25—H25	118.9
C9—C10—C11	119.5 (3)	C24—C25—H25	118.9
C9—C10—H10	120.2	N4—C26—C22	123.9 (3)
C11—C10—H10	120.2	N4—C26—H26	118.1
C12—C11—C10	119.5 (3)	C22—C26—H26	118.1
C12—C11—C13	120.8 (3)	C5—N1—C1	118.4 (3)
C10—C11—C13	119.6 (3)	C5—N1—Zn1^{i}	120.4 (2)
C11—C12—C6	121.1 (3)	C1—N1—Zn1^{i}	121.1 (2)
C11—C12—H12	119.4	C13—N2—N3	106.3 (2)
C6—C12—H12	119.4	C14—N3—N2	105.9 (2)
N2—C13—O1	113.0 (3)	C26—N4—C25	118.0 (3)
N2—C13—C11	129.6 (3)	C26—N4—Zn1	120.5 (2)
O1—C13—C11	117.4 (3)	C25—N4—Zn1	121.4 (2)
N3—C14—O1	112.3 (3)	C13—O1—C14	102.5 (2)
N3—C14—C15	130.1 (3)	N1^{ii}—Zn1—N4	100.39 (10)
O1—C14—C15	117.5 (3)	N1^{ii}—Zn1—Cl1	111.14 (8)
C21—C15—C16	119.2 (3)	N4—Zn1—Cl1	105.91 (7)

C21—C15—C14	120.2 (3)	N1^{ii}—Zn1—Cl2	107.72 (8)
C16—C15—C14	120.7 (3)	N4—Zn1—Cl2	108.18 (7)
C17—C16—C15	119.5 (3)	Cl1—Zn1—Cl2	121.42 (4)
C17—C16—H16	120.3		

N1—C1—C2—C3	−3.0 (6)	C19—C18—C20—C22	6.0 (5)
C1—C2—C3—C4	−0.4 (6)	C16—C15—C21—C20	−2.2 (5)
C2—C3—C4—C5	3.5 (5)	C14—C15—C21—C20	177.0 (3)
C2—C3—C4—C6	−177.4 (3)	C18—C20—C21—C15	0.2 (5)
C3—C4—C5—N1	−3.6 (5)	C22—C20—C21—C15	179.2 (3)
C6—C4—C5—N1	177.2 (3)	C21—C20—C22—C26	−55.0 (4)
C3—C4—C6—C12	−51.4 (4)	C18—C20—C22—C26	124.0 (3)
C5—C4—C6—C12	127.7 (3)	C21—C20—C22—C23	123.3 (3)
C3—C4—C6—C7	126.2 (4)	C18—C20—C22—C23	−57.6 (4)
C5—C4—C6—C7	−54.7 (4)	C26—C22—C23—C24	−2.2 (5)
C12—C6—C7—C9	−0.1 (5)	C20—C22—C23—C24	179.4 (3)
C4—C6—C7—C9	−177.7 (3)	C22—C23—C24—C25	0.5 (5)
C12—C6—C7—C8	178.3 (3)	C23—C24—C25—N4	1.0 (5)
C4—C6—C7—C8	0.7 (5)	C23—C22—C26—N4	2.7 (5)
C6—C7—C9—C10	−0.1 (5)	C20—C22—C26—N4	−178.9 (3)
C8—C7—C9—C10	−178.6 (3)	C4—C5—N1—C1	0.4 (5)
C7—C9—C10—C11	−0.3 (5)	C4—C5—N1—Zn1^{i}	−178.5 (2)
C9—C10—C11—C12	1.0 (5)	C2—C1—N1—C5	3.0 (5)
C9—C10—C11—C13	178.6 (3)	C2—C1—N1—Zn1^{i}	−178.1 (3)
C10—C11—C12—C6	−1.2 (5)	O1—C13—N2—N3	1.2 (3)
C13—C11—C12—C6	−178.8 (3)	C11—C13—N2—N3	−177.7 (3)
C7—C6—C12—C11	0.8 (5)	O1—C14—N3—N2	0.4 (3)
C4—C6—C12—C11	178.5 (3)	C15—C14—N3—N2	177.6 (3)
C12—C11—C13—N2	−176.4 (3)	C13—N2—N3—C14	−1.0 (3)
C10—C11—C13—N2	6.0 (5)	C22—C26—N4—C25	−1.2 (4)
C12—C11—C13—O1	4.7 (4)	C22—C26—N4—Zn1	177.0 (2)
C10—C11—C13—O1	−172.9 (3)	C24—C25—N4—C26	−0.7 (5)
N3—C14—C15—C21	175.3 (3)	C24—C25—N4—Zn1	−178.9 (3)
O1—C14—C15—C21	−7.6 (4)	N2—C13—O1—C14	−1.0 (3)
N3—C14—C15—C16	−5.5 (5)	C11—C13—O1—C14	178.1 (3)
O1—C14—C15—C16	171.6 (3)	N3—C14—O1—C13	0.3 (3)
C21—C15—C16—C17	1.6 (5)	C15—C14—O1—C13	−177.3 (3)
C14—C15—C16—C17	−177.6 (3)	C26—N4—Zn1—N1^{ii}	94.5 (2)
C15—C16—C17—C18	1.1 (5)	C25—N4—Zn1—N1^{ii}	−87.3 (2)
C16—C17—C18—C20	−3.1 (5)	C26—N4—Zn1—Cl1	−149.8 (2)
C16—C17—C18—C19	174.4 (3)	C25—N4—Zn1—Cl1	28.4 (3)
C17—C18—C20—C21	2.4 (4)	C26—N4—Zn1—Cl2	−18.2 (2)
C19—C18—C20—C21	−175.0 (3)	C25—N4—Zn1—Cl2	160.0 (2)
C17—C18—C20—C22	−176.6 (3)		

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