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Dichlorido(2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline)zinc(II) 0.35-hydrate

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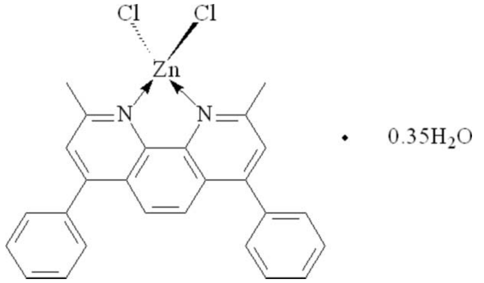
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.044; wR factor = 0.108; data-to-parameter ratio = 17.9.

The title compound, $[ZnCl_2(C_{26}H_{20}N_2)]\cdot0.35H_2O$, consists of one mononuclear dichlorido(2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline)zinc(II) molecule and a partial-occupancy water molecule. The Zn^{II} atom is coordinated by two N atoms of one phenanthroline molecule and two chloride ions in a tetrahedral geometry. In the structure there exist O—H···Cl hydrogen bonds and π–π interactions [centroid–centroid = 4.035 (4) Å and vertical distance = 3.883 (4) Å], which lead to the formation of one-dimensional supramolecular chains. This compound is isostructural with the $CuCl_2$, NiI_2, $NiBr_2$ and PtI_2 adducts of the ligand 9-dimethyl-4,7-diphenyl-1,10-phenanthroline.

Related literature

For related literature, see: Butcher & Sinn (1977); Fanizzi *et al.* (1996); Green *et al.* (1984); Kinnunen *et al.* (2000); Klemens *et al.* (1989); Muniz & Nieger (2006); Sun *et al.* (2001); Wall *et al.* (1999); Wang *et al.* (2007).



Experimental

Crystal data

$[ZnCl_2(C_{26}H_{20}N_2)]\cdot0.35H_2O$
M_r = 503.02
Monoclinic, $P2_1/c$
a = 13.052 (3) Å
b = 22.350 (5) Å
c = 8.0698 (16) Å
β = 103.39 (3)°
V = 2290.1 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.645, T_{max} = 0.672
22571 measured reflections
5246 independent reflections
3836 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.01
5246 reflections
293 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···Cl1	0.85	2.28	3.049 (10)	150
O1W—H1WB···Cl2^{i}	0.85	2.26	3.091 (10)	167

Symmetry code: (i) $x, y, z-1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2039).

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supplementary materials

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Dichlorido(2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline)zinc(II) 0.35-hydrate

Y.-E. Qiu

Comment

The crystal structures of 9-dimethyl-4,7-diphenyl-1,10-phenanthroline (Wang *et al.*, 2007) and its some metal complexes have been documented (Butcher & Sinn, 1977; Fanizzi *et al.*, 1996; Green *et al.*, 1984; Kinnunen *et al.*, 2000; Klemens *et al.*, 1989; Muniz & Nieger, 2006; Sun *et al.*, 2001; Wall *et al.*, 1999 and Wang *et al.*, 2007), which feature mononuclear structure. pi π The title compound, $Zn(C_{26}H_{20}N_2)Cl_2·0.35H_2O$ (I) consists of mono-nuclear $Zn(C_{26}H_{20}N_2)Cl_2$ molecules and packing water molecules (Fig. 1). The center Zn^{II} atom locates on a normal position and is coordinated by two N atoms of one phenanthroline molecule and two chloride ions to form a tetrahedral geometry, with the bond distances and angles being normal. The dihedral angles between two benzene rings and phenanthroline ring are 39.4 (4)° and 45.8 (4)°, respectively. Furthermore, in the structure there exist O—H—Cl hydrogen bonds (Table 2) and weak π-π interactions [between rings C11—C14—C25—C26 and C11A—C14A—C25A—C26A (symmetry code for A: x, $1/2 - y$, $1/2 + z$); the centro-centro distance is 4.035 (4) Å, vertical distance is 3.883 (4)Å and dihedral angel is 22.3 (4)°] which lead to the formation of one-dimensional supramolecular chains arranged along the c direction (Fig. 2).

This compound is isostructural with the $CuCl_2$, $NiBr_2$, NiI_2 and PtI_2 adducts of the ligand, 9-dimethyl-4,7-diphenyl-1,10-phenanthroline (Butcher & Sinn, 1977; Fanizzi *et al.*, Kinnunen *et al.*, 2000 and Wall *et al.*, 1999).

Experimental

A mixture of 9-dimethyl-4,7-diphenyl-1,10-phenanthroline (36 mg, 0.1 mmol), $ZnCl_2$ (27 mg, 0.2 mmol) and terephthalic acid (17 mg, 0.1 mmol) in water/ethanol (8 ml, $V_{5:1}$) was sealed in a Teflon-lined stainless-steel Parr bomb that was heated at 443 K for 48 h. Yellow crystals of (I) were collected after the bomb was allowed to cool to room temperature over 36 h. The yield is 30% with respect to 9-dimethyl-4,7-diphenyl-1,10-phenanthroline.

Refinement

H atoms of organic ligands were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 or 0.96Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C,N). The s.o.f of water O atom was obtained in the refinement as 0.35 and so, the s.o.f parameters of the whole aquous molecule were kept fiked as 0.35 in the final refinement. The H atoms of water molecules were located in Fourier difference map and refined with bond restraints O—H = 0.85 (1) Å, and with U_{iso}(H) = 1.2 U_{eq} (O).

Figures

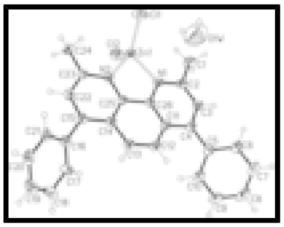

Fig. 1. Displacement ellipsoid plot (30% probability) of the structure of (I).

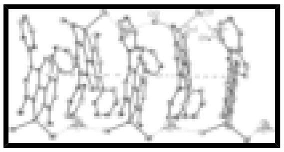

Fig. 2. one-dimensional packing of molecules in (I) showing O—H—Cl hydrogen bonds and π-π interactions.

Dichlorido(2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline)zinc(II) 0.35-hydrate

Crystal data

$[ZnCl_2(C_{26}H_{20}N_2)]\cdot 0.35H_2O$	F_{000} = 1030
M_r = 503.02	D_x = 1.460 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 18099 reflections
a = 13.052 (3) Å	θ = 3.2–27.6º
b = 22.350 (5) Å	μ = 1.32 mm^{-1}
c = 8.0698 (16) Å	T = 293 (2) K
β = 103.39 (3)º	Block, colorless
V = 2290.1 (9) Å^3	0.40 × 0.30 × 0.30 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	5246 independent reflections
Radiation source: fine-focus sealed tube	3836 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.2º
Absorption correction: Multi-Scan (SADABS; Bruker, 1998)	$h = -16\rightarrow16$
T_{min} = 0.645, T_{max} = 0.672	$k = -29\rightarrow29$
22571 measured reflections	$l = -10\rightarrow10$

Refinement

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

$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 1.2738P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
5246 reflections	$\Delta\rho_{max} = 0.55$ e Å^{-3}
293 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Zn1	0.24140 (2)	0.425932 (13)	0.91197 (4)	0.04537 (12)	
N1	0.13155 (16)	0.36139 (9)	0.8123 (3)	0.0406 (5)	
N2	0.33832 (16)	0.35180 (9)	0.9449 (3)	0.0382 (5)	
C1	−0.0159 (3)	0.43068 (13)	0.7480 (5)	0.0703 (10)	
H1A	0.0052	0.4478	0.8598	0.106*	
H1B	−0.0914	0.4288	0.7147	0.106*	
H1C	0.0099	0.4550	0.6685	0.106*	
C2	0.0288 (2)	0.36850 (12)	0.7496 (4)	0.0449 (6)	
C3	−0.0352 (2)	0.31954 (12)	0.6906 (4)	0.0454 (6)	
H3A	−0.1070	0.3257	0.6484	0.054*	
C4	0.0040 (2)	0.26217 (11)	0.6925 (3)	0.0402 (6)	
C5	−0.0698 (2)	0.21172 (12)	0.6376 (4)	0.0439 (6)	
C6	−0.1541 (2)	0.21785 (14)	0.4980 (4)	0.0514 (7)	
H6A	−0.1630	0.2536	0.4371	0.062*	
C7	−0.2252 (2)	0.17162 (17)	0.4476 (5)	0.0661 (9)	
H7A	−0.2809	0.1762	0.3531	0.079*	
C8	−0.2130 (3)	0.11838 (16)	0.5389 (6)	0.0734 (11)	
H8A	−0.2598	0.0870	0.5045	0.088*	
C9	−0.1316 (3)	0.11233 (14)	0.6801 (5)	0.0694 (10)	
H9A	−0.1245	0.0771	0.7431	0.083*	
C10	−0.0601 (2)	0.15829 (13)	0.7292 (4)	0.0539 (7)	
H10A	−0.0049	0.1535	0.8244	0.065*	

C11	0.11470 (19)	0.25453 (11)	0.7525 (3)	0.0361 (5)	
C12	0.1703 (2)	0.19917 (11)	0.7515 (3)	0.0425 (6)	
H12A	0.1335	0.1657	0.7014	0.051*	
C13	0.2741 (2)	0.19432 (11)	0.8208 (4)	0.0427 (6)	
H13A	0.3066	0.1574	0.8192	0.051*	
C14	0.33589 (19)	0.24435 (11)	0.8971 (3)	0.0364 (6)	
C15	0.4453 (2)	0.24203 (11)	0.9772 (3)	0.0396 (6)	
C16	0.5051 (2)	0.18483 (11)	1.0058 (3)	0.0414 (6)	
C17	0.4670 (3)	0.13535 (13)	1.0770 (4)	0.0533 (7)	
H17A	0.4020	0.1375	1.1055	0.064*	
C18	0.5248 (3)	0.08287 (14)	1.1058 (4)	0.0640 (9)	
H18A	0.4984	0.0500	1.1531	0.077*	
C19	0.6214 (3)	0.07928 (14)	1.0643 (4)	0.0657 (9)	
H19A	0.6605	0.0441	1.0839	0.079*	
C20	0.6595 (2)	0.12777 (15)	0.9944 (4)	0.0589 (8)	
H20A	0.7243	0.1253	0.9654	0.071*	
C21	0.6025 (2)	0.18061 (13)	0.9663 (4)	0.0482 (7)	
H21A	0.6299	0.2135	0.9205	0.058*	
C22	0.4954 (2)	0.29529 (12)	1.0305 (3)	0.0437 (6)	
H22A	0.5673	0.2949	1.0790	0.052*	
C23	0.4414 (2)	0.34995 (11)	1.0139 (3)	0.0424 (6)	
C24	0.4954 (2)	0.40787 (13)	1.0754 (4)	0.0577 (8)	
H24A	0.4821	0.4365	0.9843	0.087*	
H24B	0.5699	0.4012	1.1124	0.087*	
H24C	0.4689	0.4229	1.1688	0.087*	
C25	0.28637 (19)	0.30029 (10)	0.8873 (3)	0.0353 (5)	
C26	0.17432 (19)	0.30565 (10)	0.8140 (3)	0.0345 (5)	
Cl1	0.27868 (8)	0.48510 (4)	0.71742 (13)	0.0771 (3)	
Cl2	0.21894 (8)	0.46162 (4)	1.15462 (11)	0.0745 (3)	
O1W	0.1051 (9)	0.4306 (5)	0.4394 (13)	0.137 (4)	0.35
H1WA	0.1338 (9)	0.4472 (5)	0.5341 (15)	0.165*	0.35
H1WB	0.1301 (9)	0.4445 (5)	0.3590 (14)	0.165*	0.35

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0496 (2)	0.02520 (15)	0.0623 (2)	−0.00321 (13)	0.01503 (16)	−0.00313 (14)
N1	0.0415 (12)	0.0298 (10)	0.0522 (13)	−0.0019 (9)	0.0143 (10)	−0.0037 (9)
N2	0.0397 (12)	0.0279 (10)	0.0469 (12)	−0.0045 (9)	0.0099 (10)	−0.0036 (9)
C1	0.0489 (17)	0.0406 (16)	0.119 (3)	0.0074 (14)	0.0142 (19)	−0.0041 (18)
C2	0.0400 (14)	0.0377 (14)	0.0587 (17)	0.0030 (11)	0.0152 (13)	−0.0008 (12)
C3	0.0345 (13)	0.0439 (15)	0.0584 (17)	−0.0002 (11)	0.0118 (13)	−0.0023 (13)
C4	0.0393 (14)	0.0397 (14)	0.0438 (15)	−0.0042 (11)	0.0140 (12)	−0.0046 (11)
C5	0.0399 (14)	0.0455 (15)	0.0507 (16)	−0.0077 (11)	0.0194 (13)	−0.0120 (12)
C6	0.0425 (15)	0.0564 (17)	0.0573 (18)	−0.0043 (13)	0.0159 (14)	−0.0123 (14)
C7	0.0433 (17)	0.077 (2)	0.076 (2)	−0.0097 (16)	0.0107 (16)	−0.0324 (19)
C8	0.0519 (19)	0.058 (2)	0.114 (3)	−0.0193 (16)	0.026 (2)	−0.034 (2)
C9	0.065 (2)	0.0414 (17)	0.109 (3)	−0.0102 (15)	0.033 (2)	−0.0080 (18)

C10	0.0502 (17)	0.0440 (16)	0.070 (2)	−0.0082 (13)	0.0199 (15)	−0.0072 (14)
C11	0.0361 (13)	0.0336 (12)	0.0405 (14)	−0.0035 (10)	0.0126 (11)	−0.0057 (10)
C12	0.0435 (15)	0.0328 (13)	0.0526 (16)	−0.0052 (11)	0.0138 (13)	−0.0134 (11)
C13	0.0473 (15)	0.0283 (12)	0.0542 (16)	0.0021 (11)	0.0154 (13)	−0.0081 (11)
C14	0.0397 (14)	0.0302 (12)	0.0405 (14)	0.0029 (10)	0.0116 (12)	−0.0028 (10)
C15	0.0423 (14)	0.0375 (13)	0.0393 (14)	0.0033 (11)	0.0101 (12)	−0.0019 (11)
C16	0.0449 (15)	0.0375 (14)	0.0402 (14)	0.0052 (11)	0.0066 (12)	−0.0041 (11)
C17	0.0637 (19)	0.0450 (16)	0.0550 (18)	0.0087 (14)	0.0214 (15)	0.0028 (13)
C18	0.090 (3)	0.0425 (17)	0.059 (2)	0.0114 (16)	0.0156 (19)	0.0071 (14)
C19	0.078 (2)	0.0503 (19)	0.059 (2)	0.0253 (17)	−0.0029 (18)	−0.0074 (15)
C20	0.0421 (16)	0.069 (2)	0.0606 (19)	0.0143 (15)	0.0009 (15)	−0.0153 (16)
C21	0.0436 (15)	0.0491 (16)	0.0484 (16)	0.0014 (12)	0.0033 (13)	−0.0076 (13)
C22	0.0382 (14)	0.0421 (14)	0.0470 (16)	−0.0007 (11)	0.0019 (12)	−0.0011 (12)
C23	0.0454 (15)	0.0341 (13)	0.0462 (15)	−0.0060 (11)	0.0077 (13)	−0.0018 (11)
C24	0.0515 (17)	0.0376 (15)	0.076 (2)	−0.0094 (13)	−0.0015 (16)	−0.0051 (14)
C25	0.0384 (13)	0.0303 (12)	0.0389 (14)	−0.0022 (10)	0.0122 (11)	−0.0043 (10)
C26	0.0379 (13)	0.0285 (11)	0.0388 (13)	−0.0002 (10)	0.0124 (11)	−0.0031 (10)
Cl1	0.0892 (6)	0.0537 (5)	0.1020 (7)	0.0040 (4)	0.0498 (6)	0.0240 (5)
Cl2	0.1134 (8)	0.0447 (4)	0.0694 (5)	0.0036 (4)	0.0291 (5)	−0.0131 (4)
O1W	0.156 (9)	0.166 (11)	0.094 (7)	−0.058 (8)	0.037 (7)	−0.009 (6)

Geometric parameters (Å, °)

Zn1—N1	2.062 (2)	C11—C12	1.435 (3)
Zn1—N2	2.064 (2)	C12—C13	1.345 (4)
Zn1—Cl1	2.1918 (9)	C12—H12A	0.9300
Zn1—Cl2	2.1960 (10)	C13—C14	1.432 (3)
N1—C2	1.329 (3)	C13—H13A	0.9300
N1—C26	1.364 (3)	C14—C25	1.401 (3)
N2—C23	1.332 (3)	C14—C15	1.425 (4)
N2—C25	1.362 (3)	C15—C22	1.378 (4)
C1—C2	1.506 (4)	C15—C16	1.488 (3)
C1—H1A	0.9600	C16—C21	1.384 (4)
C1—H1B	0.9600	C16—C17	1.390 (4)
C1—H1C	0.9600	C17—C18	1.385 (4)
C2—C3	1.392 (4)	C17—H17A	0.9300
C3—C4	1.379 (4)	C18—C19	1.380 (5)
C3—H3A	0.9300	C18—H18A	0.9300
C4—C11	1.424 (3)	C19—C20	1.367 (5)
C4—C5	1.483 (4)	C19—H19A	0.9300
C5—C6	1.387 (4)	C20—C21	1.386 (4)
C5—C10	1.395 (4)	C20—H20A	0.9300
C6—C7	1.386 (4)	C21—H21A	0.9300
C6—H6A	0.9300	C22—C23	1.401 (4)
C7—C8	1.389 (5)	C22—H22A	0.9300
C7—H7A	0.9300	C23—C24	1.503 (4)
C8—C9	1.373 (5)	C24—H24A	0.9600
C8—H8A	0.9300	C24—H24B	0.9600
C9—C10	1.382 (4)	C24—H24C	0.9600

C9—H9A	0.9300	C25—C26	1.450 (3)
C10—H10A	0.9300	O1W—H1WA	0.8535
C11—C26	1.407 (3)	O1W—H1WB	0.8497

N1—Zn1—N2	80.71 (8)	C13—C12—H12A	119.0
N1—Zn1—Cl1	113.10 (7)	C11—C12—H12A	119.0
N2—Zn1—Cl1	110.20 (7)	C12—C13—C14	121.9 (2)
N1—Zn1—Cl2	112.20 (7)	C12—C13—H13A	119.0
N2—Zn1—Cl2	112.41 (7)	C14—C13—H13A	119.0
Cl1—Zn1—Cl2	121.15 (4)	C25—C14—C15	117.3 (2)
C2—N1—C26	119.2 (2)	C25—C14—C13	117.8 (2)
C2—N1—Zn1	127.90 (17)	C15—C14—C13	124.9 (2)
C26—N1—Zn1	112.90 (16)	C22—C15—C14	117.6 (2)
C23—N2—C25	119.4 (2)	C22—C15—C16	120.0 (2)
C23—N2—Zn1	127.46 (16)	C14—C15—C16	122.4 (2)
C25—N2—Zn1	113.12 (16)	C21—C16—C17	118.5 (2)
C2—C1—H1A	109.5	C21—C16—C15	120.0 (2)
C2—C1—H1B	109.5	C17—C16—C15	121.5 (2)
H1A—C1—H1B	109.5	C18—C17—C16	120.7 (3)
C2—C1—H1C	109.5	C18—C17—H17A	119.7
H1A—C1—H1C	109.5	C16—C17—H17A	119.7
H1B—C1—H1C	109.5	C19—C18—C17	120.1 (3)
N1—C2—C3	120.6 (2)	C19—C18—H18A	119.9
N1—C2—C1	117.9 (2)	C17—C18—H18A	119.9
C3—C2—C1	121.5 (2)	C20—C19—C18	119.6 (3)
C4—C3—C2	122.4 (2)	C20—C19—H19A	120.2
C4—C3—H3A	118.8	C18—C19—H19A	120.2
C2—C3—H3A	118.8	C19—C20—C21	120.7 (3)
C3—C4—C11	117.4 (2)	C19—C20—H20A	119.6
C3—C4—C5	119.3 (2)	C21—C20—H20A	119.6
C11—C4—C5	123.3 (2)	C16—C21—C20	120.5 (3)
C6—C5—C10	118.2 (3)	C16—C21—H21A	119.8
C6—C5—C4	120.4 (3)	C20—C21—H21A	119.8
C10—C5—C4	121.3 (3)	C15—C22—C23	122.1 (2)
C7—C6—C5	121.0 (3)	C15—C22—H22A	118.9
C7—C6—H6A	119.5	C23—C22—H22A	118.9
C5—C6—H6A	119.5	N2—C23—C22	120.3 (2)
C6—C7—C8	119.8 (3)	N2—C23—C24	117.6 (2)
C6—C7—H7A	120.1	C22—C23—C24	122.1 (2)
C8—C7—H7A	120.1	C23—C24—H24A	109.5
C9—C8—C7	119.7 (3)	C23—C24—H24B	109.5
C9—C8—H8A	120.1	H24A—C24—H24B	109.5
C7—C8—H8A	120.1	C23—C24—H24C	109.5
C8—C9—C10	120.4 (3)	H24A—C24—H24C	109.5
C8—C9—H9A	119.8	H24B—C24—H24C	109.5
C10—C9—H9A	119.8	N2—C25—C14	123.2 (2)
C9—C10—C5	120.8 (3)	N2—C25—C26	116.4 (2)
C9—C10—H10A	119.6	C14—C25—C26	120.3 (2)
C5—C10—H10A	119.6	N1—C26—C11	123.1 (2)
C26—C11—C4	117.2 (2)	N1—C26—C25	116.8 (2)

C26—C11—C12	117.6 (2)	C11—C26—C25	120.0 (2)
C4—C11—C12	125.2 (2)	H1WA—O1W—H1WB	111.0
C13—C12—C11	121.9 (2)		

N2—Zn1—N1—C2	179.0 (2)	C25—C14—C15—C16	175.9 (2)
Cl1—Zn1—N1—C2	−72.9 (2)	C13—C14—C15—C16	−6.5 (4)
Cl2—Zn1—N1—C2	68.5 (2)	C22—C15—C16—C21	−46.7 (4)
N2—Zn1—N1—C26	−1.11 (17)	C14—C15—C16—C21	133.9 (3)
Cl1—Zn1—N1—C26	106.99 (17)	C22—C15—C16—C17	131.2 (3)
Cl2—Zn1—N1—C26	−111.63 (17)	C14—C15—C16—C17	−48.1 (4)
N1—Zn1—N2—C23	−179.3 (2)	C21—C16—C17—C18	−0.7 (4)
Cl1—Zn1—N2—C23	69.4 (2)	C15—C16—C17—C18	−178.7 (3)
Cl2—Zn1—N2—C23	−69.0 (2)	C16—C17—C18—C19	0.2 (5)
N1—Zn1—N2—C25	0.58 (17)	C17—C18—C19—C20	−0.2 (5)
Cl1—Zn1—N2—C25	−110.73 (17)	C18—C19—C20—C21	0.7 (5)
Cl2—Zn1—N2—C25	110.86 (17)	C17—C16—C21—C20	1.2 (4)
C26—N1—C2—C3	1.8 (4)	C15—C16—C21—C20	179.2 (3)
Zn1—N1—C2—C3	−178.4 (2)	C19—C20—C21—C16	−1.2 (5)
C26—N1—C2—C1	−179.5 (3)	C14—C15—C22—C23	2.5 (4)
Zn1—N1—C2—C1	0.4 (4)	C16—C15—C22—C23	−176.9 (3)
N1—C2—C3—C4	−0.6 (4)	C25—N2—C23—C22	−1.4 (4)
C1—C2—C3—C4	−179.3 (3)	Zn1—N2—C23—C22	178.47 (19)
C2—C3—C4—C11	−2.1 (4)	C25—N2—C23—C24	179.9 (2)
C2—C3—C4—C5	176.2 (3)	Zn1—N2—C23—C24	−0.3 (4)
C3—C4—C5—C6	40.6 (4)	C15—C22—C23—N2	0.0 (4)
C11—C4—C5—C6	−141.1 (3)	C15—C22—C23—C24	178.6 (3)
C3—C4—C5—C10	−136.0 (3)	C23—N2—C25—C14	0.2 (4)
C11—C4—C5—C10	42.3 (4)	Zn1—N2—C25—C14	−179.64 (19)
C10—C5—C6—C7	−1.7 (4)	C23—N2—C25—C26	179.9 (2)
C4—C5—C6—C7	−178.4 (3)	Zn1—N2—C25—C26	0.0 (3)
C5—C6—C7—C8	0.6 (5)	C15—C14—C25—N2	2.2 (4)
C6—C7—C8—C9	1.1 (5)	C13—C14—C25—N2	−175.5 (2)
C7—C8—C9—C10	−1.7 (5)	C15—C14—C25—C26	−177.4 (2)
C8—C9—C10—C5	0.6 (5)	C13—C14—C25—C26	4.8 (4)
C6—C5—C10—C9	1.1 (4)	C2—N1—C26—C11	−0.1 (4)
C4—C5—C10—C9	177.7 (3)	Zn1—N1—C26—C11	−179.98 (19)
C3—C4—C11—C26	3.6 (4)	C2—N1—C26—C25	−178.7 (2)
C5—C4—C11—C26	−174.7 (2)	Zn1—N1—C26—C25	1.5 (3)
C3—C4—C11—C12	−175.0 (3)	C4—C11—C26—N1	−2.6 (4)
C5—C4—C11—C12	6.7 (4)	C12—C11—C26—N1	176.1 (2)
C26—C11—C12—C13	6.1 (4)	C4—C11—C26—C25	175.9 (2)
C4—C11—C12—C13	−175.4 (3)	C12—C11—C26—C25	−5.4 (4)
C11—C12—C13—C14	−1.2 (4)	N2—C25—C26—N1	−1.0 (3)
C12—C13—C14—C25	−4.3 (4)	C14—C25—C26—N1	178.7 (2)
C12—C13—C14—C15	178.1 (3)	N2—C25—C26—C11	−179.6 (2)
C25—C14—C15—C22	−3.5 (4)	C14—C25—C26—C11	0.1 (4)
C13—C14—C15—C22	174.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···Cl1	0.85	2.28	3.049 (10)	150
O1W—H1WB···Cl2^{i}	0.85	2.26	3.091 (10)	167

Symmetry codes: (i) x, y, z−1.

Fig. 1

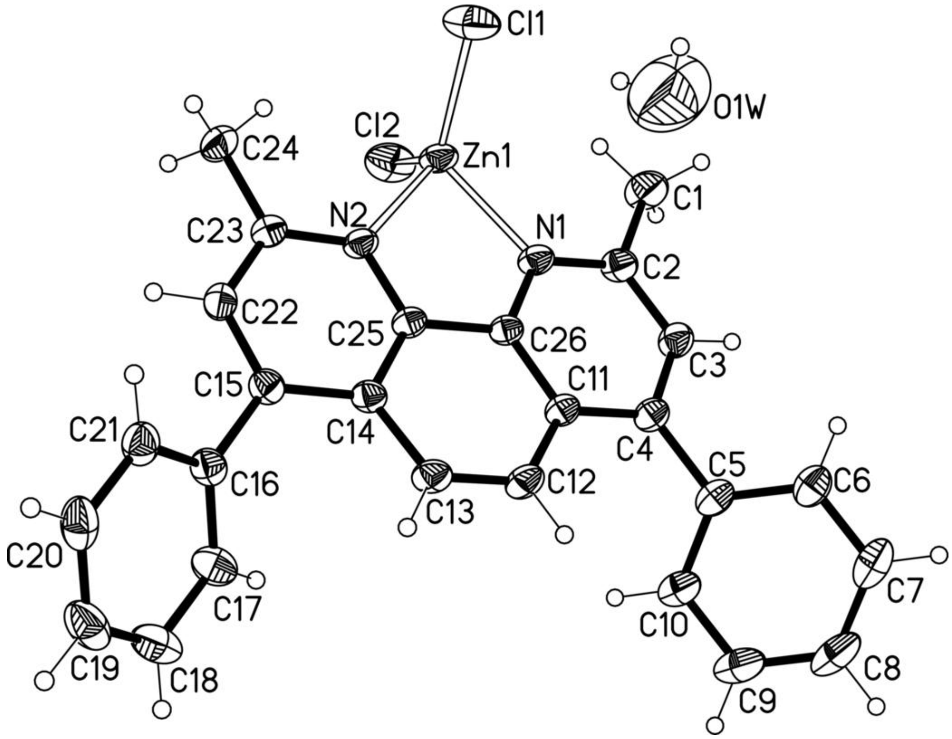
Cl1
O1W
Cl2
Zn1
C24
C1
C23
N2
N1
C2
C22
C25
C26
C3
C15
C11
C21
C14
C4
C5
C6
C16
C13
C12
C20
C7
C17
C10
C19
C18
C8
C9

Fig. 2