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2-(2-Furyl)-1*H*-imidazo[4,5-*f*][1,10]-phenanthroline-3,7-diium dichloride monohydrate

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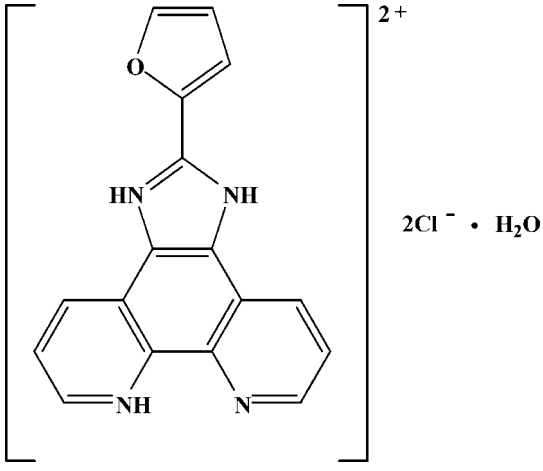
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.115; data-to-parameter ratio = 12.7.

The organic cation of the title salt, $C_{17}H_{12}N_4O^{2+}\cdot 2Cl^-\cdot H_2O$, is nearly planar, the dihedral angle between two pyridine rings being 2.53 (16)° and that between the pyridinum and furan rings being 4.17 (19)°. Molecules are linked *via* N—H···O, N—H···Cl and O—H···Cl hydrogen bonds, forming a three-dimensional framework and π–π stacking interactions help to stabilize the crystal structure [the imidazole–pyridine and imidazole–benzene centroid–centroid distances are 3.501 (3) and 3.674 (3) Å; respectively].

Related literature

For general background, see: Zhao *et al.* (2004); Zheng *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{12}N_4O^{2+}\cdot 2Cl^-\cdot H_2O$
M_r = 377.22
Monoclinic, $P2_1/n$
a = 4.768 (3) Å
b = 17.897 (10) Å
c = 19.241 (11) Å
β = 92.060 (8)°
V = 1641.0 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 293 (2) K
0.23 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.911, T_{max} = 0.940
10782 measured reflections
2859 independent reflections
1886 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.115
S = 1.02
2859 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1W	0.86	1.76	2.618 (3)	177
N2—H2A···Cl1	0.86	2.12	2.981 (3)	179
N4—H4···Cl2^{i}	0.86	2.33	3.103 (3)	150
O1W—H1WA···Cl2^{ii}	1.02	2.00	3.011 (3)	172
O1W—H1WB···Cl2^{iii}	0.93	2.19	3.112 (3)	173

Symmetry codes: (i) $x+1, y, z$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2707).

References

Bruker, (2005). APPEX2, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhao, Y. J., Xue, S. F., Zhu, Q. J., Tao, Z., Zhang, J. X., Wei, Z. B., Long, L. S., Hu, M. L., Xiao, H. P. & Day, A. I. (2004). *Chin. Sci. Bull.* **49**, 1111–1116.
Zheng, L. M., Zhu, J. N., Zhang, Y. Q., Tao, Z., Xue, S. F., Zhu, Q. J., Wei, Z. B. & Long, L. S. (2005). *Chin. J. Inorg. Chem.* **21**, 1583–1588.

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2-(2-Furyl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-3,7-diium dichloride monohydrate

Ming-Hua Chen, Yun-Qian Zhang, Qian-Jiang Zhu, Sai-Feng Xue and Zhu Tao

S1. Comment

Recent year, we used different alkyl-substituted glycolurils as the building blocks to synthesize the partially alkyl substituted cucurbit[*n*]urils (Zhao *et al.*, 2004; Zheng *et al.*, 2005). In this work, we further report the crystal structure of a phenanthroline-substituted semi-glycoluril.

The molecular structure of the title compound (I), consists of organic cations, two Cl^- anions and one water molecule (Fig. 1). The organic cation is nearly planar, the dihedral angle between two pyridine rings is 2.53 (16) ° and that one between N4-pyridine ring and furan ring is 4.17 (19)°. Molecules are linked *via* N1—H1A···O1W, N2—H2A···Cl1, N4—H4···Cl2, O1W—H1WA···Cl2 and O1W—H1WB···Cl2 hydrogen bonds (Table 1) forming a three-dimensional framework. In additional, the $\pi\cdots\pi$ stacking interaction occurs between adjacent organic cations, the centroid-to-centroid distance of *Cg*2 to *Cg*3^{iv} is 3.501 (3)Å and *Cg*2 to *Cg*5^{iv} is 3.674 (3)Å [*Cg*2, *Cg*3 and *Cg*5 is the centroid of the N1-imidazole ring, N3-pyridine ring and C6-benzene ring, respectively. Symmerty codes: (iv) -1 + *x*, *y*, *z*].

S2. Experimental

1,10-Phenanthroline-5,6-dione (1.0 g, 4.75 mmol) and ammonium acetate (3.9 g, 5 mmol) are dissolved in acetic acid glacial (60 mL) at 333 K, after cooling at room temperature, we can get lots of yellow deposits by the neutrlizing with ammonia to pH = 8–9 after 4 h of mixing with furaldhyde (0.8 mL) at 353 K. After the recryslalization in ethanol, the yellow product was dissolved in the dilute hydrochloric acid and red-brown crystals were obtained

after ten days.

S3. Refinement

Water H atoms were located in a difference Fourier synthesis and refined riding in their as-found positions relative to O atoms with U_{iso}(H) =1.2U_{eq}(O). All other H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, N—H = 0.86 Å, and with U_{iso}(H) = 1.2 U_{eq} (C, N).

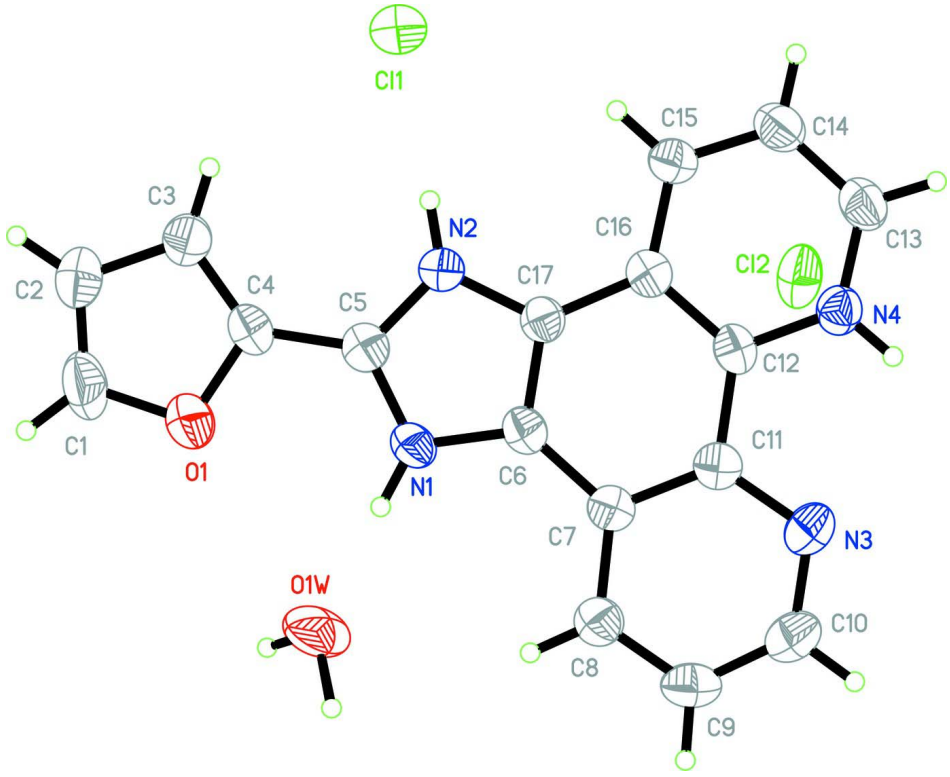

Figure 1

The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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$b = 17.897\ (10)$ Å
$c = 19.241\ (11)$ Å
$\beta = 92.060\ (8)°$
$V = 1641.0\ (16)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.527$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2859 reflections
$\theta = 1.6–25.0°$
$\mu = 0.42$ mm^{-1}
$T = 293$ K
Prism, red-brown
0.23 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.911$, $T_{max} = 0.940$
10782 measured reflections
2859 independent reflections
1886 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -5\rightarrow5$
$k = -20\rightarrow21$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.115$
$S = 1.02$
2859 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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	0.2549 (7)	0.5257 (2)	0.91899 (18)	0.0595 (10)
H1	0.1981	0.5270	0.9647	0.071*
C2	0.1543 (7)	0.57043 (18)	0.86872 (17)	0.0491 (9)
H2	0.0184	0.6073	0.8728	0.059*
C3	0.2960 (6)	0.55060 (16)	0.80743 (16)	0.0439 (8)
H3	0.2711	0.5718	0.7635	0.053*
C4	0.4742 (6)	0.49469 (16)	0.82609 (15)	0.0366 (7)
C5	0.6721 (6)	0.45050 (15)	0.78964 (15)	0.0356 (7)
C6	0.9978 (6)	0.36694 (15)	0.76729 (14)	0.0334 (7)
C7	1.2049 (6)	0.30919 (15)	0.77145 (14)	0.0331 (7)
C8	1.2878 (6)	0.26901 (16)	0.83160 (16)	0.0405 (8)
H8	1.2062	0.2786	0.8739	0.049*
C9	1.4924 (6)	0.21529 (17)	0.82645 (16)	0.0465 (8)
H9	1.5506	0.1877	0.8653	0.056*
C10	1.6108 (6)	0.20276 (16)	0.76279 (17)	0.0453 (8)
H10	1.7500	0.1665	0.7607	0.054*
C11	1.3351 (6)	0.29168 (15)	0.70909 (14)	0.0328 (7)
C12	1.2531 (6)	0.33026 (15)	0.64536 (14)	0.0320 (7)
C13	1.3161 (6)	0.34323 (16)	0.52471 (15)	0.0417 (8)
H13	1.4109	0.3287	0.4855	0.050*
C14	1.1068 (6)	0.39700 (16)	0.51891 (15)	0.0420 (8)
H14	1.0577	0.4177	0.4758	0.050*
C15	0.9734 (6)	0.41932 (15)	0.57711 (14)	0.0376 (7)
H15	0.8349	0.4559	0.5741	0.045*
C16	1.0477 (6)	0.38639 (15)	0.64198 (14)	0.0322 (7)

C17	0.9259 (6)	0.40383 (15)	0.70643 (14)	0.0319 (7)
N3	1.5391 (5)	0.23910 (13)	0.70414 (13)	0.0412 (6)
N4	1.3821 (5)	0.31224 (12)	0.58612 (12)	0.0359 (6)
H4	1.5130	0.2792	0.5882	0.043*
N1	0.8358 (5)	0.39716 (13)	0.81854 (11)	0.0348 (6)
H1A	0.8394	0.3840	0.8615	0.042*
N2	0.7228 (5)	0.45605 (12)	0.72179 (12)	0.0345 (6)
H2A	0.6432	0.4867	0.6928	0.041*
O1	0.4528 (5)	0.47741 (12)	0.89489 (11)	0.0550 (6)
Cl1	0.44997 (17)	0.56432 (4)	0.62293 (4)	0.0514 (3)
Cl2	0.83425 (17)	0.20341 (5)	0.53339 (5)	0.0579 (3)
O1W	0.8356 (5)	0.35229 (14)	0.94806 (11)	0.0703 (8)
H1WA	0.9993	0.3370	0.9803	0.084*
H1WB	0.6840	0.3400	0.9751	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (2)	0.077 (3)	0.049 (2)	0.008 (2)	0.0175 (18)	−0.016 (2)
C2	0.047 (2)	0.046 (2)	0.055 (2)	0.0040 (16)	0.0111 (17)	−0.0081 (17)
C3	0.048 (2)	0.0404 (19)	0.044 (2)	0.0041 (16)	0.0072 (16)	0.0008 (15)
C4	0.0363 (17)	0.0435 (18)	0.0304 (17)	−0.0035 (15)	0.0052 (14)	−0.0034 (14)
C5	0.0371 (18)	0.0338 (17)	0.0360 (19)	−0.0036 (14)	0.0023 (14)	−0.0014 (13)
C6	0.0325 (16)	0.0372 (17)	0.0307 (17)	−0.0030 (14)	0.0030 (13)	−0.0017 (13)
C7	0.0321 (16)	0.0339 (17)	0.0331 (18)	−0.0038 (13)	0.0004 (13)	0.0010 (13)
C8	0.0395 (18)	0.0436 (19)	0.0387 (18)	0.0014 (15)	0.0033 (14)	0.0035 (15)
C9	0.051 (2)	0.046 (2)	0.042 (2)	0.0001 (16)	−0.0055 (16)	0.0126 (15)
C10	0.0442 (19)	0.0371 (19)	0.054 (2)	0.0061 (15)	−0.0062 (17)	−0.0002 (16)
C11	0.0309 (16)	0.0328 (17)	0.0344 (18)	−0.0052 (13)	−0.0028 (13)	−0.0023 (13)
C12	0.0302 (16)	0.0345 (17)	0.0314 (17)	−0.0060 (13)	0.0043 (13)	−0.0048 (13)
C13	0.049 (2)	0.0446 (19)	0.0318 (18)	−0.0005 (16)	0.0065 (15)	−0.0037 (14)
C14	0.053 (2)	0.0402 (19)	0.0327 (18)	−0.0001 (16)	0.0047 (15)	0.0011 (14)
C15	0.0422 (18)	0.0368 (18)	0.0339 (18)	0.0011 (14)	0.0025 (14)	0.0043 (14)
C16	0.0331 (16)	0.0308 (16)	0.0329 (17)	−0.0045 (13)	0.0019 (13)	−0.0018 (13)
C17	0.0332 (16)	0.0310 (16)	0.0314 (17)	−0.0010 (13)	0.0010 (13)	−0.0022 (13)
N3	0.0389 (15)	0.0349 (15)	0.0497 (17)	0.0050 (12)	−0.0006 (12)	−0.0030 (12)
N4	0.0351 (14)	0.0377 (15)	0.0349 (15)	0.0019 (11)	0.0009 (11)	−0.0045 (11)
N1	0.0371 (14)	0.0396 (15)	0.0281 (14)	−0.0006 (12)	0.0062 (11)	0.0040 (11)
N2	0.0364 (14)	0.0356 (14)	0.0315 (15)	0.0042 (11)	0.0023 (11)	0.0033 (11)
O1	0.0560 (15)	0.0699 (16)	0.0400 (14)	0.0159 (12)	0.0122 (11)	0.0021 (11)
Cl1	0.0573 (5)	0.0518 (5)	0.0452 (5)	0.0106 (4)	0.0014 (4)	0.0082 (4)
Cl2	0.0407 (5)	0.0682 (6)	0.0651 (6)	0.0031 (4)	0.0057 (4)	−0.0194 (5)
O1W	0.0487 (15)	0.120 (2)	0.0432 (14)	0.0106 (14)	0.0133 (11)	0.0309 (14)

Geometric parameters (Å, º)

C1—C2	1.332 (4)	C10—N3	1.336 (4)
C1—O1	1.373 (4)	C10—H10	0.9300

C1—H1	0.9300	C11—N3	1.359 (3)
C2—C3	1.425 (4)	C11—C12	1.449 (4)
C2—H2	0.9300	C12—N4	1.353 (3)
C3—C4	1.353 (4)	C12—C16	1.403 (4)
C3—H3	0.9300	C13—N4	1.333 (3)
C4—O1	1.367 (3)	C13—C14	1.388 (4)
C4—C5	1.434 (4)	C13—H13	0.9300
C5—N2	1.340 (3)	C14—C15	1.367 (4)
C5—N1	1.341 (3)	C14—H14	0.9300
C6—C17	1.377 (4)	C15—C16	1.414 (4)
C6—N1	1.384 (3)	C15—H15	0.9300
C6—C7	1.429 (4)	C16—C17	1.423 (4)
C7—C11	1.406 (4)	C17—N2	1.385 (3)
C7—C8	1.407 (4)	N4—H4	0.8600
C8—C9	1.376 (4)	N1—H1A	0.8600
C8—H8	0.9300	N2—H2A	0.8600
C9—C10	1.385 (4)	O1W—H1WA	1.0173
C9—H9	0.9300	O1W—H1WB	0.9323

C2—C1—O1	111.5 (3)	C7—C11—C12	120.1 (3)
C2—C1—H1	124.2	N4—C12—C16	118.0 (3)
O1—C1—H1	124.2	N4—C12—C11	118.8 (3)
C1—C2—C3	106.4 (3)	C16—C12—C11	123.2 (3)
C1—C2—H2	126.8	N4—C13—C14	120.4 (3)
C3—C2—H2	126.8	N4—C13—H13	119.8
C4—C3—C2	106.1 (3)	C14—C13—H13	119.8
C4—C3—H3	127.0	C15—C14—C13	119.4 (3)
C2—C3—H3	127.0	C15—C14—H14	120.3
C3—C4—O1	110.9 (3)	C13—C14—H14	120.3
C3—C4—C5	134.1 (3)	C14—C15—C16	119.5 (3)
O1—C4—C5	115.0 (3)	C14—C15—H15	120.3
N2—C5—N1	109.5 (3)	C16—C15—H15	120.3
N2—C5—C4	125.5 (3)	C12—C16—C15	119.5 (3)
N1—C5—C4	125.0 (3)	C12—C16—C17	115.0 (2)
C17—C6—N1	106.9 (2)	C15—C16—C17	125.5 (3)
C17—C6—C7	123.0 (3)	C6—C17—N2	107.3 (2)
N1—C6—C7	130.1 (3)	C6—C17—C16	122.6 (3)
C11—C7—C8	117.9 (3)	N2—C17—C16	130.1 (2)
C11—C7—C6	116.0 (2)	C10—N3—C11	116.1 (3)
C8—C7—C6	126.1 (3)	C13—N4—C12	123.2 (3)
C9—C8—C7	118.5 (3)	C13—N4—H4	118.4
C9—C8—H8	120.8	C12—N4—H4	118.4
C7—C8—H8	120.8	C5—N1—C6	108.3 (2)
C8—C9—C10	119.3 (3)	C5—N1—H1A	125.8
C8—C9—H9	120.3	C6—N1—H1A	125.8
C10—C9—H9	120.3	C5—N2—C17	108.1 (2)
N3—C10—C9	124.6 (3)	C5—N2—H2A	126.0
N3—C10—H10	117.7	C17—N2—H2A	126.0

C9—C10—H10	117.7	C4—O1—C1	105.1 (2)
N3—C11—C7	123.6 (3)	H1WA—O1W—H1WB	100.9
N3—C11—C12	116.3 (3)		

O1—C1—C2—C3	−0.3 (4)	C11—C12—C16—C17	0.8 (4)
C1—C2—C3—C4	−0.2 (4)	C14—C15—C16—C12	−1.3 (4)
C2—C3—C4—O1	0.5 (3)	C14—C15—C16—C17	−179.7 (3)
C2—C3—C4—C5	179.6 (3)	N1—C6—C17—N2	0.3 (3)
C3—C4—C5—N2	−0.9 (5)	C7—C6—C17—N2	−179.4 (2)
O1—C4—C5—N2	178.1 (3)	N1—C6—C17—C16	−178.8 (2)
C3—C4—C5—N1	178.9 (3)	C7—C6—C17—C16	1.4 (4)
O1—C4—C5—N1	−2.0 (4)	C12—C16—C17—C6	−1.9 (4)
C17—C6—C7—C11	0.2 (4)	C15—C16—C17—C6	176.6 (3)
N1—C6—C7—C11	−179.5 (3)	C12—C16—C17—N2	179.2 (3)
C17—C6—C7—C8	−179.7 (3)	C15—C16—C17—N2	−2.3 (5)
N1—C6—C7—C8	0.6 (5)	C9—C10—N3—C11	0.0 (4)
C11—C7—C8—C9	0.4 (4)	C7—C11—N3—C10	0.9 (4)
C6—C7—C8—C9	−179.6 (3)	C12—C11—N3—C10	−178.9 (2)
C7—C8—C9—C10	0.4 (4)	C14—C13—N4—C12	0.2 (4)
C8—C9—C10—N3	−0.6 (5)	C16—C12—N4—C13	−2.5 (4)
C8—C7—C11—N3	−1.1 (4)	C11—C12—N4—C13	178.2 (2)
C6—C7—C11—N3	179.0 (2)	N2—C5—N1—C6	−0.2 (3)
C8—C7—C11—C12	178.7 (2)	C4—C5—N1—C6	179.9 (3)
C6—C7—C11—C12	−1.3 (4)	C17—C6—N1—C5	−0.1 (3)
N3—C11—C12—N4	−0.2 (4)	C7—C6—N1—C5	179.6 (3)
C7—C11—C12—N4	180.0 (2)	N1—C5—N2—C17	0.4 (3)
N3—C11—C12—C16	−179.4 (2)	C4—C5—N2—C17	−179.7 (3)
C7—C11—C12—C16	0.8 (4)	C6—C17—N2—C5	−0.4 (3)
N4—C13—C14—C15	1.6 (4)	C16—C17—N2—C5	178.6 (3)
C13—C14—C15—C16	−1.0 (4)	C3—C4—O1—C1	−0.7 (3)
N4—C12—C16—C15	3.0 (4)	C5—C4—O1—C1	−180.0 (3)
C11—C12—C16—C15	−177.8 (2)	C2—C1—O1—C4	0.6 (4)
N4—C12—C16—C17	−178.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1*W*	0.86	1.76	2.618 (3)	177
N2—H2*A*···Cl1	0.86	2.12	2.981 (3)	179
N4—H4···Cl2^{i}	0.86	2.33	3.103 (3)	150
O1*W*—H1*WA*···Cl2^{ii}	1.02	2.00	3.011 (3)	172
O1*W*—H1*WB*···Cl2^{iii}	0.93	2.19	3.112 (3)	173

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