Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-Ethylenedibenzimidazolium dichloride tetrahydrate

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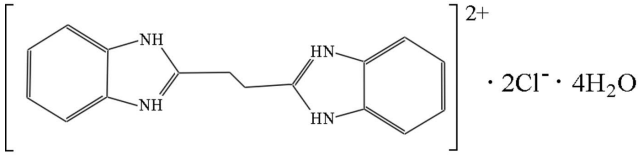
Received 11 April 2007; accepted 26 June 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.105; data-to-parameter ratio = 14.0.

In the title compound, $C_{16}H_{16}N_4^{2+}\cdot 2Cl^-\cdot 4H_2O$, the molecules and ions are linked through N—H···Cl, O—H···Cl, O—H···O and N—H···O hydrogen bonds, while π–π stacking interactions between benzimidazolium units [the centroid-to-centroid distances between stacking benzene rings are 3.635 (3) and 3.817 (3) Å, respectively] and an N—H···π interaction help to stabilize the crystal structure.

Related literature

For related literature, see: Day & Arnold (2000); Day *et al.* (2002); Freeman *et al.* (1981); Kim *et al.* (2000); Wang & Joullié (1957).



Experimental

Crystal data

$C_{16}H_{16}N_4^{2+}\cdot 2Cl^-\cdot 4H_2O$
M_r = 407.29
Triclinic, $P\overline{1}$
a = 7.174 (6) Å
b = 9.652 (8) Å
c = 15.411 (13) Å
α = 80.504 (8)°
β = 79.684 (9)°
γ = 68.520 (8)°
V = 971.2 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 293 (2) K
0.17 × 0.14 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick,1997)
T_{min} = 0.941, T_{max} = 0.972
6584 measured reflections
3317 independent reflections
2933 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.105
S = 1.09
3317 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	1.86	2.719 (2)	178
N2—H2A···Cl1^{ii}	0.86	2.41	3.201 (2)	152
N3—H3A···Cl2	0.86	2.26	3.104 (3)	165
N4—H4A···O1	0.86	1.87	2.711 (3)	167
O1—H1A···O3	0.92	1.90	2.798 (3)	166
O1—H1B···Cl2^{iii}	0.95	2.34	3.216 (2)	152
O2—H2B···O4^{iv}	0.89	1.93	2.790 (3)	164
O2—H2C···Cl1	0.95	2.31	3.208 (2)	156
O3—H3B···Cl1	0.99	2.26	3.249 (3)	174
O3—H3C···Cl1^{iv}	0.90	2.41	3.310 (3)	176
O4—H4B···Cl2^{v}	0.95	2.35	3.300 (3)	174
O4—H4C···Cl2^{vi}	0.90	2.50	3.383 (3)	169
N1—H1···$Cg3^{vii}$	0.86	3.40	3.354 (3)	80

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Natural Science Foundation of China (No. 20662003), the 'Chun-Hui' Fund of Chinese Ministry of Education, the International Collaborative Project of Guizhou Province (No. 2007400108) and the Governor Foundation of Guizhou Province.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2080).

References

Bruker (2002). *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 1.22. Bruker AXS Inc., Madison, Wisconsin, USA.
Day, A. I. & Arnold, A. P. (2000). Int. Patent WO 2000 068 232.
Day, A. I., Blanch, R. J., Arnold, A. P., Lorenzo, S., Lewis, G. R. & Dance, I. (2002). *Angew. Chem. Int. Ed.* **41**, 275–277.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Freeman, W. A., Mock, W. L. & Shih, N. Y. (1981). *J. Am. Chem. Soc.* **103**, 7367–7368.
Kim, J., Jung, I.-S., Kim, S.-Y., Lee, E., Kang, J.-K., Sakamoto, S., Yamaguchi, K. & Kim, K. (2000). *J. Am. Chem. Soc.* **122**, 540–541.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, L. L.-Y. & Joullié, M. M. (1957). *J. Am. Chem. Soc.* **79**, 5706–5708.

  doi:10.1107/S1600536807031273

supplementary materials

Acta Cryst. (2007). E**63**, o3578 [**doi:10.1107/S1600536807031273**]

2,2'-Ethylenedibenzimidazolium dichloride tetrahydrate

J.-M. Yi, Y.-Q. Zhang, S.-F. Xue, Q.-J. Zhu and Z. Tao

Comment

We present an 'axle' type polyaromatic compound (I) that contains multiple functional groups that can develop strong intermolecular interactions with cucurbit[*n*]urils (CB[*n*]) (Freeman *et al.*, 1981; Day & Arnold, 2000; Day *et al.*, 2002; Kim *et al.*, 2000).

The molecular structure of (I), shown in Fig. 1, consists of an organic cation, Cl^- anions and lattice water molecules. The two benzimidazolyl rings in the organic cation are not co-planar, with a dihedral angle of 27.77 (6)° between them. Molecules are linked *via* a network of hydrogen bonds (N1—H1···O2, O2—H2C···Cl1, N2—H2A···Cl1, N3—H3A···Cl2, O1—H1B···Cl2, N4—H4A···O1, O1—H1A···O3, O3—H3B···Cl1; Table 1).

π···π stacking interactions are observed between nearly parallel benzimidazolyl benzene rings. The centroid-to-centroid distance between C1–C6 benzene rings is 3.635 (3) Å (symmetry code: –*X*,-Y,1-*Z*), while between C11–C16 benzene rings it is 3.817 (3) Å (symmetry codes:1-*X*,1-Y,-*Z*). In addition, an N—H···π interaction occurs between adjacent benzimidazolyl groups, with an N1—H1···*Cg*(3) angle of 79.89°, and H1···*Cg*(3) and N1···*Cg*(3) distances of 3.3964Å and 3.354 (3) Å, respectively [*Cg*(3) is the centroid of the C1–C6-benzene (symmetry codes:1-*X*,-Y,1-*Z*)].

Experimental

o-Phenylenediamine (5.40 g, 0.05 mol) and succinic acid (2.95 g, 0.025 mol) were refluxed for twelve hours in 50 mL of 4*M* HCl. The reaction mixture was then cooled for one day and the blue crystalline dihydrochloride was removed by filtration and dried. Crystals of the dihydrochloride suitable for X-ray diffraction were obtained by dissolving in water and allowing the solution to stand at room temperature for several days (Wang *et al.*, 1957). Yield: 43%.

Refinement

Water H atoms were located in a difference Fourier synthesis and refined 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).

Figures

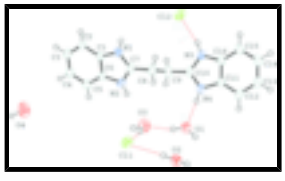


Fig. 1. The molecular structure of (I), shown with the atom numbering scheme and 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

2,2'-Ethylenedibenzimidazolium dichloride tetrahydrate

Crystal data

$C_{16}H_{16}N_4^{2+}\cdot 2Cl^-\cdot 4H_2O$	$Z = 2$
$M_r = 407.29$	$F_{000} = 428$
Triclinic, $P\overline{1}$	$D_x = 1.393$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.174$ (6) Å	Cell parameters from 3317 reflections
$b = 9.652$ (8) Å	$\theta = 1.4$–25.0º
$c = 15.411$ (13) Å	$\mu = 0.36$ mm^{-1}
$\alpha = 80.504$ (8)º	$T = 293$ (2) K
$\beta = 79.684$ (9)º	Prism, colourless
$\gamma = 68.520$ (8)º	0.17 × 0.14 × 0.08 mm
$V = 971.2$ (14) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3317 independent reflections
Radiation source: fine-focus sealed tube	2933 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.4$º
Absorption correction: multi-scan (SADABS; Sheldrick,1997)	$h = -8\rightarrow 8$
$T_{min} = 0.941$, $T_{max} = 0.972$	$k = -11\rightarrow 11$
6584 measured reflections	$l = -16\rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.105$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.2765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
3317 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.27$ 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. 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}
C1	0.6983 (2)	1.03103 (18)	0.52524 (10)	0.0288 (3)
C2	0.6639 (3)	1.16652 (19)	0.47131 (12)	0.0359 (4)
H2	0.5807	1.2572	0.4920	0.043*
C3	0.7605 (3)	1.1583 (2)	0.38534 (12)	0.0385 (4)
H3	0.7424	1.2464	0.3473	0.046*
C4	0.8855 (3)	1.0215 (2)	0.35315 (11)	0.0391 (4)
H4	0.9459	1.0212	0.2945	0.047*
C5	0.9199 (3)	0.8880 (2)	0.40694 (12)	0.0374 (4)
H5	1.0028	0.7974	0.3861	0.045*
C6	0.8248 (2)	0.89511 (18)	0.49381 (11)	0.0302 (4)
C7	0.7063 (2)	0.84969 (19)	0.63476 (11)	0.0357 (4)
C8	0.6641 (3)	0.7702 (2)	0.72354 (13)	0.0472 (5)
H8A	0.6060	0.6970	0.7165	0.057*
H8B	0.5654	0.8419	0.7610	0.057*
C9	0.8508 (3)	0.6921 (2)	0.76849 (12)	0.0480 (5)
H9A	0.9461	0.6159	0.7328	0.058*
H9B	0.9136	0.7641	0.7721	0.058*
C10	0.8068 (3)	0.6206 (2)	0.85950 (11)	0.0367 (4)
C11	0.7655 (2)	0.45577 (18)	0.97231 (11)	0.0300 (4)
C12	0.7552 (3)	0.32862 (19)	1.02773 (12)	0.0373 (4)
H12	0.7750	0.2396	1.0055	0.045*
C13	0.7139 (3)	0.3424 (2)	1.11733 (12)	0.0427 (4)
H13	0.7079	0.2596	1.1567	0.051*
C14	0.6805 (3)	0.4770 (2)	1.15129 (12)	0.0435 (5)
H14	0.6515	0.4812	1.2123	0.052*
C15	0.6896 (3)	0.6028 (2)	1.09654 (12)	0.0402 (4)
H15	0.6663	0.6924	1.1188	0.048*
C16	0.7356 (2)	0.58891 (18)	1.00602 (11)	0.0312 (4)
N1	0.6283 (2)	0.99668 (16)	0.61347 (9)	0.0330 (3)
H1	0.5477	1.0603	0.6485	0.040*
N2	0.8250 (2)	0.78573 (15)	0.56483 (10)	0.0369 (3)
H2A	0.8914	0.6915	0.5638	0.044*
N3	0.7621 (2)	0.68854 (16)	0.93284 (9)	0.0367 (3)

H3A	0.7512	0.7798	0.9347	0.044*
N4	0.8080 (2)	0.48110 (16)	0.88072 (9)	0.0352 (3)
H4A	0.8312	0.4171	0.8438	0.042*
O1	0.8156 (2)	0.29177 (16)	0.76720 (9)	0.0541 (4)
H1A	0.7466	0.3352	0.7192	0.065*
H1B	0.7641	0.2151	0.7953	0.065*
O2	0.3755 (2)	0.19384 (16)	0.72672 (9)	0.0550 (4)
H2B	0.3037	0.1536	0.7691	0.066*
H2C	0.2837	0.2748	0.6944	0.066*
O3	0.6201 (3)	0.46531 (18)	0.62377 (10)	0.0628 (4)
H3B	0.4915	0.4593	0.6121	0.122 (12)*
H3C	0.6796	0.4806	0.5679	0.107 (11)*
O4	0.7843 (3)	0.9552 (2)	0.12510 (12)	0.0885 (6)
H4B	0.9091	0.9725	0.1156	0.106*
H4C	0.7735	0.9600	0.0675	0.106*
Cl1	0.18700 (7)	0.47137 (5)	0.58431 (3)	0.05045 (17)
Cl2	0.76500 (10)	1.01372 (6)	0.90382 (4)	0.0651 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0309 (8)	0.0306 (8)	0.0258 (8)	−0.0118 (7)	−0.0047 (6)	−0.0015 (6)
C2	0.0413 (9)	0.0278 (9)	0.0378 (10)	−0.0107 (7)	−0.0078 (8)	−0.0018 (7)
C3	0.0463 (10)	0.0361 (9)	0.0349 (10)	−0.0198 (8)	−0.0104 (8)	0.0092 (7)
C4	0.0426 (10)	0.0504 (11)	0.0266 (9)	−0.0221 (8)	−0.0011 (7)	0.0000 (8)
C5	0.0364 (9)	0.0363 (9)	0.0364 (10)	−0.0105 (7)	0.0026 (7)	−0.0085 (8)
C6	0.0297 (8)	0.0285 (8)	0.0309 (9)	−0.0103 (7)	−0.0036 (6)	0.0013 (7)
C7	0.0309 (9)	0.0392 (10)	0.0323 (9)	−0.0110 (7)	−0.0039 (7)	0.0056 (7)
C8	0.0406 (10)	0.0528 (12)	0.0389 (11)	−0.0150 (9)	−0.0013 (8)	0.0136 (9)
C9	0.0447 (11)	0.0604 (13)	0.0349 (10)	−0.0207 (9)	−0.0035 (8)	0.0101 (9)
C10	0.0339 (9)	0.0419 (10)	0.0322 (9)	−0.0139 (8)	−0.0061 (7)	0.0053 (8)
C11	0.0278 (8)	0.0336 (9)	0.0280 (8)	−0.0110 (7)	−0.0038 (6)	−0.0007 (7)
C12	0.0350 (9)	0.0315 (9)	0.0440 (11)	−0.0122 (7)	−0.0044 (7)	0.0009 (8)
C13	0.0373 (10)	0.0435 (11)	0.0402 (11)	−0.0138 (8)	−0.0026 (8)	0.0124 (8)
C14	0.0407 (10)	0.0581 (12)	0.0261 (9)	−0.0144 (9)	−0.0010 (7)	0.0008 (8)
C15	0.0437 (10)	0.0432 (10)	0.0354 (10)	−0.0147 (8)	−0.0059 (8)	−0.0089 (8)
C16	0.0313 (8)	0.0325 (9)	0.0318 (9)	−0.0140 (7)	−0.0073 (7)	0.0016 (7)
N1	0.0343 (7)	0.0344 (8)	0.0267 (7)	−0.0093 (6)	−0.0010 (6)	−0.0027 (6)
N2	0.0365 (8)	0.0255 (7)	0.0391 (8)	−0.0055 (6)	0.0001 (6)	0.0047 (6)
N3	0.0455 (8)	0.0307 (7)	0.0359 (8)	−0.0182 (6)	−0.0060 (6)	0.0035 (6)
N4	0.0392 (8)	0.0383 (8)	0.0277 (8)	−0.0134 (6)	−0.0027 (6)	−0.0038 (6)
O1	0.0742 (10)	0.0461 (8)	0.0385 (8)	−0.0168 (7)	−0.0033 (7)	−0.0088 (6)
O2	0.0685 (9)	0.0482 (8)	0.0396 (8)	−0.0106 (7)	−0.0032 (7)	−0.0074 (6)
O3	0.0675 (10)	0.0706 (11)	0.0457 (9)	−0.0211 (8)	−0.0100 (7)	0.0020 (7)
O4	0.1155 (16)	0.1051 (15)	0.0603 (11)	−0.0637 (13)	−0.0186 (10)	0.0163 (10)
Cl1	0.0523 (3)	0.0349 (3)	0.0540 (3)	−0.0059 (2)	−0.0056 (2)	−0.0004 (2)
Cl2	0.0916 (4)	0.0397 (3)	0.0694 (4)	−0.0299 (3)	−0.0209 (3)	0.0068 (3)

Geometric parameters (Å, °)

C1—N1	1.393 (2)	C11—C12	1.393 (3)
C1—C2	1.393 (2)	C11—C16	1.395 (3)
C1—C6	1.400 (2)	C12—C13	1.377 (3)
C2—C3	1.381 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.404 (3)
C3—C4	1.409 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.375 (3)
C4—C5	1.376 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.392 (3)
C5—C6	1.390 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—N3	1.390 (2)
C6—N2	1.389 (2)	N1—H1	0.8600
C7—N1	1.328 (2)	N2—H2A	0.8600
C7—N2	1.332 (2)	N3—H3A	0.8600
C7—C8	1.493 (3)	N4—H4A	0.8600
C8—C9	1.504 (3)	O1—H1A	0.9193
C8—H8A	0.9700	O1—H1B	0.9531
C8—H8B	0.9700	O2—H2B	0.8859
C9—C10	1.491 (3)	O2—H2C	0.9513
C9—H9A	0.9700	O3—H3B	0.9944
C9—H9B	0.9700	O3—H3C	0.9044
C10—N4	1.330 (3)	O4—H4B	0.9517
C10—N3	1.331 (2)	O4—H4C	0.8972
C11—N4	1.390 (2)		
N1—C1—C2	131.94 (15)	N3—C10—C9	124.31 (18)
N1—C1—C6	106.44 (14)	N4—C11—C12	131.65 (16)
C2—C1—C6	121.62 (16)	N4—C11—C16	106.66 (15)
C3—C2—C1	116.08 (16)	C12—C11—C16	121.67 (16)
C3—C2—H2	122.0	C13—C12—C11	116.09 (17)
C1—C2—H2	122.0	C13—C12—H12	122.0
C2—C3—C4	122.42 (16)	C11—C12—H12	122.0
C2—C3—H3	118.8	C12—C13—C14	122.31 (17)
C4—C3—H3	118.8	C12—C13—H13	118.8
C5—C4—C3	121.21 (17)	C14—C13—H13	118.8
C5—C4—H4	119.4	C15—C14—C13	121.59 (18)
C3—C4—H4	119.4	C15—C14—H14	119.2
C4—C5—C6	116.86 (16)	C13—C14—H14	119.2
C4—C5—H5	121.6	C14—C15—C16	116.44 (17)
C6—C5—H5	121.6	C14—C15—H15	121.8
N2—C6—C5	132.39 (16)	C16—C15—H15	121.8
N2—C6—C1	105.81 (15)	N3—C16—C15	132.35 (16)
C5—C6—C1	121.80 (16)	N3—C16—C11	105.79 (15)
N1—C7—N2	109.51 (15)	C15—C16—C11	121.87 (16)
N1—C7—C8	124.61 (16)	C7—N1—C1	108.89 (14)
N2—C7—C8	125.88 (17)	C7—N1—H1	125.6
C7—C8—C9	112.55 (16)	C1—N1—H1	125.6

C7—C8—H8A	109.1	C7—N2—C6	109.36 (15)
C9—C8—H8A	109.1	C7—N2—H2A	125.3
C7—C8—H8B	109.1	C6—N2—H2A	125.3
C9—C8—H8B	109.1	C10—N3—C16	109.32 (15)
H8A—C8—H8B	107.8	C10—N3—H3A	125.3
C10—C9—C8	112.61 (16)	C16—N3—H3A	125.3
C10—C9—H9A	109.1	C10—N4—C11	108.79 (14)
C8—C9—H9A	109.1	C10—N4—H4A	125.6
C10—C9—H9B	109.1	C11—N4—H4A	125.6
C8—C9—H9B	109.1	H1A—O1—H1B	105.9
H9A—C9—H9B	107.8	H2B—O2—H2C	107.8
N4—C10—N3	109.43 (15)	H3B—O3—H3C	101.2
N4—C10—C9	126.25 (17)	H4B—O4—H4C	95.8
N1—C1—C2—C3	179.91 (17)	C14—C15—C16—C11	1.7 (3)
C6—C1—C2—C3	0.4 (2)	N4—C11—C16—N3	−0.14 (17)
C1—C2—C3—C4	0.5 (3)	C12—C11—C16—N3	178.47 (15)
C2—C3—C4—C5	−1.0 (3)	N4—C11—C16—C15	179.97 (15)
C3—C4—C5—C6	0.4 (3)	C12—C11—C16—C15	−1.4 (3)
C4—C5—C6—N2	179.99 (17)	N2—C7—N1—C1	0.24 (19)
C4—C5—C6—C1	0.6 (3)	C8—C7—N1—C1	−179.21 (17)
N1—C1—C6—N2	−0.16 (18)	C2—C1—N1—C7	−179.59 (18)
C2—C1—C6—N2	179.45 (15)	C6—C1—N1—C7	−0.04 (18)
N1—C1—C6—C5	179.38 (15)	N1—C7—N2—C6	−0.4 (2)
C2—C1—C6—C5	−1.0 (3)	C8—C7—N2—C6	179.10 (17)
N1—C7—C8—C9	−117.7 (2)	C5—C6—N2—C7	−179.16 (19)
N2—C7—C8—C9	62.9 (3)	C1—C6—N2—C7	0.31 (19)
C7—C8—C9—C10	176.41 (17)	N4—C10—N3—C16	1.00 (19)
C8—C9—C10—N4	90.8 (2)	C9—C10—N3—C16	−178.32 (16)
C8—C9—C10—N3	−90.0 (2)	C15—C16—N3—C10	179.36 (18)
N4—C11—C12—C13	178.22 (17)	C11—C16—N3—C10	−0.51 (18)
C16—C11—C12—C13	0.0 (2)	N3—C10—N4—C11	−1.08 (19)
C11—C12—C13—C14	1.1 (3)	C9—C10—N4—C11	178.22 (16)
C12—C13—C14—C15	−0.8 (3)	C12—C11—N4—C10	−177.67 (17)
C13—C14—C15—C16	−0.6 (3)	C16—C11—N4—C10	0.74 (18)
C14—C15—C16—N3	−178.17 (18)		

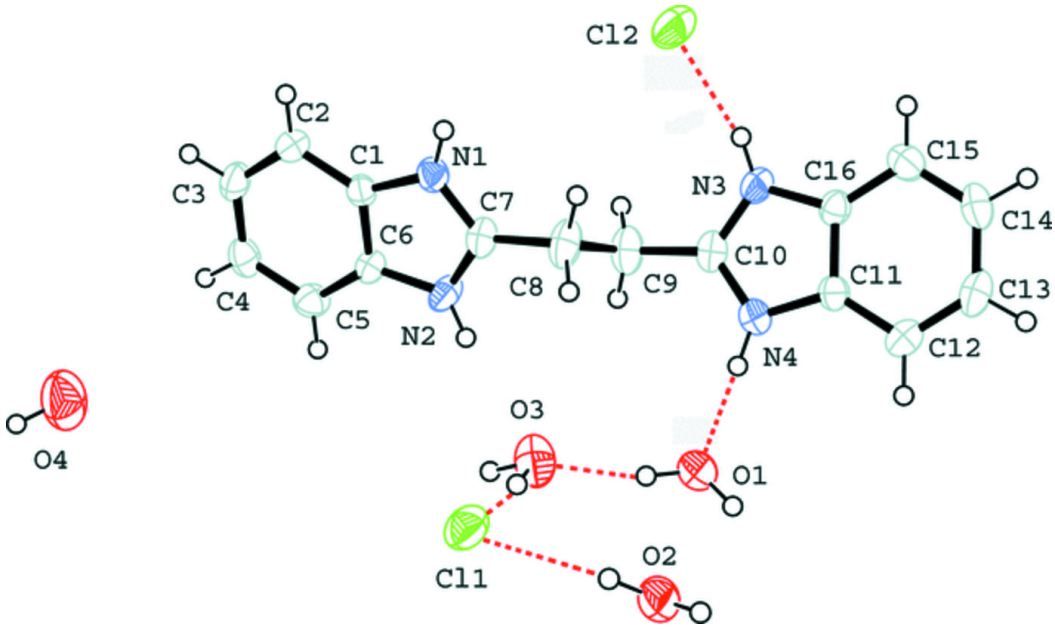
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	1.86	2.719 (2)	178
N2—H2A···Cl1^{ii}	0.86	2.41	3.201 (2)	152
N3—H3A···Cl2	0.86	2.26	3.104 (3)	165
N4—H4A···O1	0.86	1.87	2.711 (3)	167
O1—H1A···O3	0.92	1.90	2.798 (3)	166
O1—H1B···Cl2^{iii}	0.95	2.34	3.216 (2)	152
O2—H2B···O4^{iv}	0.89	1.93	2.790 (3)	164
O2—H2C···Cl1	0.95	2.31	3.208 (2)	156
O3—H3B···Cl1	0.99	2.26	3.249 (3)	174

O3—H3C···Cl1^{iv}	0.90	2.41	3.310 (3)	176
O4—H4B···Cl2^{v}	0.95	2.35	3.300 (3)	174
O4—H4C···Cl2^{vi}	0.90	2.50	3.383 (3)	169

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

Fig. 1


Cl2
C2
C1
N1
C3
C7
C6
C4
C5
N2
C8
C9
N3
C16
C15
C14
C10
C11
C13
C12
N4
O3
O1
O4
Cl1
O2