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N,*N*,*N*′,*N*′-Tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine methanol tetrasolvate dihydrate

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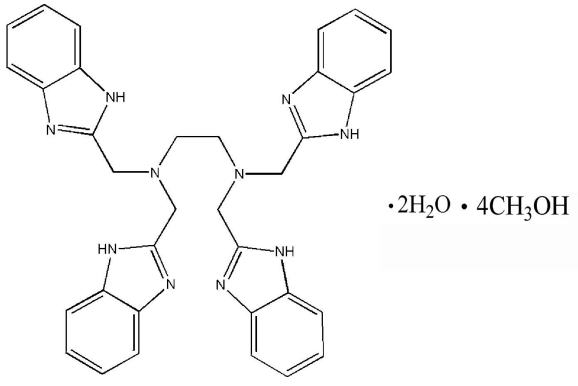
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.163; data-to-parameter ratio = 15.5.

The title compound, $C_{34}H_{32}N_{10}\cdot4CH_4O\cdot2H_2O$, crystallizes with the mid-point of the central C—C bond of the tetrabenzimidazolylethanediamine molecule located on an inversion centre. The crystal packing is stabilized by O(or N)—H···O and O—H···N hydrogen bonds.

Related literature

For related literature, see: Chen *et al.* (2004); Hendriks *et al.* (1982); Liao *et al.* (2001).



Experimental

Crystal data

$C_{34}H_{32}N_{10}\cdot4CH_4O\cdot2H_2O$
M_r = 744.90
Triclinic, $P\overline{1}$
a = 9.2349 (6) Å
b = 10.4290 (7) Å
c = 11.5344 (8) Å
α = 100.500 (1)°
β = 101.763 (1)°
γ = 99.417 (1)°
V = 1045.83 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.984, T_{max} = 0.992
10988 measured reflections
4083 independent reflections
2726 reflections with $I > 2\sigma(I)$
R_{int} = 0.094

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.163
S = 1.01
4083 reflections
264 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 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
O1—H1*C*···O2	0.87 (2)	1.85 (2)	2.702 (3)	164 (3)
O3—H3*B*···N2^{i}	0.86 (3)	1.90 (4)	2.731 (2)	163 (5)
N5—H5*A*···O1^{ii}	0.895 (19)	1.94 (2)	2.828 (2)	169.5 (19)
N3—H3*A*···O1^{ii}	0.899 (18)	1.972 (19)	2.862 (2)	170.0 (18)
O2—H2*C*···N4^{iii}	0.88 (3)	1.89 (3)	2.765 (3)	173 (5)
O1—H1*D*···O3^{iv}	0.84 (2)	1.89 (2)	2.731 (3)	177 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors are grateful for the assistance of Xianggao Meng.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2470).

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supplementary materials

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N,*N*,*N*',*N*'-Tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine methanol tetrasolvate dihydrate

Y.-M. Pei, X.-G. Meng and C.-S. Zhou

Comment

As part of our continuing studies on the ligands or metal complexes containing multi-benzimidazole groups (Chen *et al.*, 2004;Liao *et al.*,2001), we report here the crystal structure of the related title compound, which was obtained unexpectedly by reacting N,*N*,*N*', N' - tetrakis (2 '-benzimidazolyl methyl) −1,2-ethanediamine (EDTB) with Mn $(NO_3)_2 \cdot 4H_2O$ in CH_3OH and H_2O solution.

In the molecule (Fig. 1), the N2/N3/C3—C9 benzimidazole ring is twisted from the benzimidazole ring (N4/N5/C11—C17) by a dihedral angle of 47.1 (1)°. In the asymmetric unit, there is half of an EDTB molecule, two methanol and one water solvent molecules.

In the supramolecular structure, by a combination of O(or N)–H···O, and O–H···N hydrogen bonds the molecules are linked into a three-dimensional framework (Fig.2). Analysis using *PLATON* (Spek, 2003) shows that no π–π and C–H···π interactions are observed in the crystal structure.

Experimental

Chemicals of reagent grade were used without further purification. The ligand N,*N*,*N* ', N' - tetrakis (2 '-benzimidazolyl methyl) −1,2-ethanediamine (EDTB) was synthesized from reported literature earlier (Hendriks, *et al.*,1982). The title pink salt was obtained unexpectedly by reacting EDTB (0.29 g, 0.5 mmol) in 20 ml hot methanol with Mn $(NO_3)_2 \cdot 4H_2O$ (0.25 g, 1.0 mmol) solution of 10 ml H_2O. The mixture was stirred for 1 h at 303k and then filtered. The resulting pink solution was allowed to stand at room temperature for 1 week. Crystals suitale for X-ray analysis were obtained at the bottom of the vessel.

Refinement

All H atoms bonded to carbon atoms were located at their ideal positions with C–H = 0.96 Å (methyl), 0.93 Å (aromatic), 0.97 Å (methylene) and with U_{iso}(H)=1.5U_{eq}(C, methyl) or 1.2U_{eq}(C, aromatic and methylene). H atoms bonded to N and O atoms were located in difference Fourier maps and refined with distance constraints of N–H =0.86 (4) Å, O–H = 0.82 (4) Å, H–H = 1.35 (4) Å (water H) and their U_{iso} values were set 1.2 (for imine) or 1.5 (for water and hydroxyl) times that of their carrier atoms.

Figures

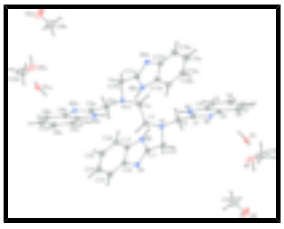

Fig. 1. View of the title molecular structure, showing 50% probability displacement ellipsoids and H atoms as small spheres. Atoms labeled with suffix 'a' are related by the symmetry operator (−*x*, −*y*, −*z* + 1).

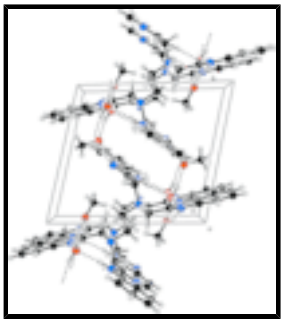

Fig. 2. Part of the crystal structure showing the formation of the three-dimensinal network. Hydrogen bonds are shown as dashed lines.

N,*N*,*N*',*N*'-Tetrakis(benzimidazol-2-ylmethyl)\ ethane-1,2-diamine methanol tetrasolvate dihydrate

Crystal data

$C_{34}H_{32}N_{10}·4CH_4O·2H_2O$	$Z = 1$
$M_r = 744.90$	$F_{000} = 398$
Triclinic, $P\overline{1}$	$D_x = 1.183$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.2349$ (6) Å	Cell parameters from 3273 reflections
$b = 10.4290$ (7) Å	$\theta = 2.3$–24.9º
$c = 11.5344$ (8) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 100.500$ (1)º	$T = 296$ (2) K
$\beta = 101.763$ (1)º	Block, pink
$\gamma = 99.417$ (1)º	0.20 × 0.20 × 0.10 mm
$V = 1045.83$ (12) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4083 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	2726 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.094$
$T = 299(2)$ K	$\theta_{max} = 26.0$º
0.3° wide ω exposures scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -10 \rightarrow 11$
$T_{min} = 0.984$, $T_{max} = 0.992$	$k = -12 \rightarrow 12$
10988 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.163$	$w = 1/[\sigma^2(F_o^2) + (0.087P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4083 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
264 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
7 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 $F^2 > 2$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	0.0644 (2)	0.05926 (17)	0.52781 (15)	0.0480 (4)
H1A	0.0399	0.1163	0.5943	0.058*
H1B	0.1549	0.0289	0.5604	0.058*
C2	0.1912 (2)	0.0801 (2)	0.36638 (17)	0.0568 (5)
H2A	0.1693	−0.0161	0.3554	0.068*
H2B	0.2955	0.1131	0.4118	0.068*
C3	0.1733 (2)	0.11411 (17)	0.24450 (16)	0.0503 (5)
C4	0.0658 (2)	0.16310 (17)	0.07461 (16)	0.0545 (5)
C5	−0.0262 (3)	0.1985 (2)	−0.01979 (18)	0.0683 (6)
H5	−0.1238	0.2093	−0.0182	0.082*
C6	0.0359 (4)	0.2169 (2)	−0.11684 (19)	0.0812 (7)
H6	−0.0208	0.2428	−0.1815	0.097*
C7	0.1793 (4)	0.1977 (3)	−0.1200 (2)	0.0887 (8)
H7	0.2159	0.2091	−0.1876	0.106*
C8	0.2696 (3)	0.1622 (2)	−0.0263 (2)	0.0758 (7)
H8	0.3660	0.1491	−0.0295	0.091*

C9	0.2119 (2)	0.14626 (18)	0.07405 (17)	0.0567 (5)
C10	0.1497 (2)	0.27781 (18)	0.49058 (18)	0.0553 (5)
H10A	0.1750	0.3237	0.4291	0.066*
H10B	0.2408	0.2903	0.5542	0.066*
C11	0.0337 (2)	0.33503 (17)	0.54216 (17)	0.0504 (5)
C12	−0.0839 (2)	0.43572 (17)	0.66124 (17)	0.0550 (5)
C13	−0.1279 (3)	0.5076 (2)	0.7564 (2)	0.0724 (6)
H13	−0.0576	0.5504	0.8287	0.087*
C14	−0.2771 (3)	0.5143 (2)	0.7419 (2)	0.0815 (7)
H14	−0.3078	0.5633	0.8048	0.098*
C15	−0.3834 (3)	0.4495 (2)	0.6349 (3)	0.0812 (7)
H15	−0.4841	0.4557	0.6277	0.097*
C16	−0.3428 (3)	0.3760 (2)	0.5389 (2)	0.0719 (6)
H16	−0.4138	0.3326	0.4671	0.086*
C17	−0.1918 (2)	0.36981 (18)	0.55440 (18)	0.0552 (5)
C18	0.4678 (4)	0.8728 (4)	0.2625 (4)	0.1300 (12)
H18A	0.5412	0.8183	0.2553	0.195*
H18B	0.3708	0.8250	0.2126	0.195*
H18C	0.4617	0.8944	0.3457	0.195*
C19	0.6472 (5)	0.4394 (4)	0.0909 (4)	0.174 (2)
H19A	0.6046	0.5171	0.1058	0.261*
H19B	0.5715	0.3674	0.0368	0.261*
H19C	0.7307	0.4586	0.0546	0.261*
N1	0.09316 (17)	0.13561 (13)	0.43655 (12)	0.0474 (4)
N2	0.27737 (18)	0.11545 (16)	0.18230 (14)	0.0581 (4)
N3	0.04414 (19)	0.14113 (15)	0.18572 (13)	0.0521 (4)
H3A	−0.040 (2)	0.151 (2)	0.2111 (18)	0.063*
N4	0.05769 (19)	0.41225 (14)	0.65166 (14)	0.0560 (4)
N5	−0.11288 (19)	0.30662 (16)	0.48112 (15)	0.0553 (4)
H5A	−0.143 (2)	0.259 (2)	0.4045 (18)	0.066*
O1	0.75915 (17)	0.17048 (18)	0.23664 (15)	0.0740 (5)
H1C	0.732 (3)	0.238 (3)	0.209 (3)	0.111*
H1D	0.682 (3)	0.114 (3)	0.236 (3)	0.111*
O2	0.6956 (3)	0.4047 (2)	0.1961 (3)	0.1419 (10)
H2C	0.771 (4)	0.468 (4)	0.242 (4)	0.213*
O3	0.5088 (2)	0.9845 (3)	0.2266 (3)	0.1536 (11)
H3B	0.444 (5)	1.036 (5)	0.228 (5)	0.230*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0588 (12)	0.0470 (9)	0.0433 (9)	0.0109 (8)	0.0137 (8)	0.0211 (7)
C2	0.0630 (13)	0.0591 (11)	0.0616 (11)	0.0201 (10)	0.0246 (10)	0.0293 (9)
C3	0.0565 (12)	0.0468 (10)	0.0556 (10)	0.0122 (8)	0.0237 (9)	0.0191 (8)
C4	0.0748 (14)	0.0404 (10)	0.0487 (10)	0.0055 (9)	0.0194 (9)	0.0117 (8)
C5	0.0903 (16)	0.0552 (12)	0.0555 (12)	0.0125 (11)	0.0105 (11)	0.0131 (10)
C6	0.126 (2)	0.0644 (14)	0.0463 (12)	0.0075 (15)	0.0132 (13)	0.0163 (10)
C7	0.127 (2)	0.0845 (17)	0.0526 (13)	−0.0038 (16)	0.0335 (15)	0.0189 (12)

C8	0.0915 (17)	0.0760 (15)	0.0612 (13)	0.0005 (12)	0.0367 (12)	0.0132 (11)
C9	0.0719 (14)	0.0471 (10)	0.0533 (11)	0.0031 (9)	0.0260 (10)	0.0126 (8)
C10	0.0591 (12)	0.0495 (10)	0.0592 (11)	0.0036 (9)	0.0151 (9)	0.0228 (9)
C11	0.0597 (13)	0.0377 (9)	0.0538 (10)	0.0040 (8)	0.0102 (9)	0.0193 (8)
C12	0.0716 (14)	0.0396 (10)	0.0559 (11)	0.0100 (9)	0.0155 (10)	0.0175 (8)
C13	0.0969 (19)	0.0534 (12)	0.0660 (13)	0.0141 (12)	0.0204 (12)	0.0115 (10)
C14	0.105 (2)	0.0613 (14)	0.0914 (18)	0.0244 (14)	0.0462 (17)	0.0193 (13)
C15	0.0784 (17)	0.0675 (14)	0.109 (2)	0.0199 (13)	0.0368 (16)	0.0287 (14)
C16	0.0683 (15)	0.0625 (13)	0.0814 (15)	0.0101 (11)	0.0125 (12)	0.0162 (11)
C17	0.0639 (13)	0.0443 (10)	0.0593 (11)	0.0101 (9)	0.0143 (10)	0.0185 (9)
C18	0.103 (2)	0.124 (3)	0.196 (4)	0.043 (2)	0.055 (2)	0.079 (3)
C19	0.165 (4)	0.112 (3)	0.186 (4)	−0.004 (2)	−0.079 (3)	0.051 (3)
N1	0.0593 (10)	0.0430 (8)	0.0477 (8)	0.0106 (7)	0.0202 (7)	0.0213 (6)
N2	0.0597 (11)	0.0605 (10)	0.0618 (10)	0.0112 (8)	0.0267 (8)	0.0206 (8)
N3	0.0592 (11)	0.0527 (9)	0.0535 (9)	0.0142 (8)	0.0237 (8)	0.0209 (7)
N4	0.0680 (11)	0.0435 (8)	0.0539 (9)	0.0069 (8)	0.0099 (8)	0.0141 (7)
N5	0.0617 (11)	0.0506 (9)	0.0496 (9)	0.0078 (8)	0.0083 (8)	0.0102 (7)
O1	0.0586 (10)	0.0798 (11)	0.0793 (10)	0.0146 (8)	0.0091 (8)	0.0155 (9)
O2	0.1251 (19)	0.0802 (13)	0.171 (2)	−0.0134 (12)	−0.0549 (16)	0.0371 (14)
O3	0.0777 (15)	0.147 (2)	0.290 (3)	0.0454 (14)	0.0767 (18)	0.128 (2)

Geometric parameters (Å, °)

C1—N1	1.471 (2)	C11—N5	1.349 (2)
C1—C1^{i}	1.508 (4)	C12—C13	1.384 (3)
C1—H1A	0.9700	C12—N4	1.391 (3)
C1—H1B	0.9700	C12—C17	1.397 (3)
C2—N1	1.452 (2)	C13—C14	1.368 (3)
C2—C3	1.495 (2)	C13—H13	0.9300
C2—H2A	0.9700	C14—C15	1.389 (4)
C2—H2B	0.9700	C14—H14	0.9300
C3—N2	1.311 (2)	C15—C16	1.381 (3)
C3—N3	1.346 (2)	C15—H15	0.9300
C4—C5	1.384 (3)	C16—C17	1.383 (3)
C4—C9	1.389 (3)	C16—H16	0.9300
C4—N3	1.390 (2)	C17—N5	1.373 (2)
C5—C6	1.386 (3)	C18—O3	1.330 (4)
C5—H5	0.9300	C18—H18A	0.9600
C6—C7	1.378 (4)	C18—H18B	0.9600
C6—H6	0.9300	C18—H18C	0.9600
C7—C8	1.372 (4)	C19—O2	1.340 (4)
C7—H7	0.9300	C19—H19A	0.9600
C8—C9	1.394 (3)	C19—H19B	0.9600
C8—H8	0.9300	C19—H19C	0.9600
C9—N2	1.389 (3)	N3—H3A	0.899 (18)
C10—N1	1.462 (2)	N5—H5A	0.895 (19)
C10—C11	1.482 (3)	O1—H1C	0.87 (2)
C10—H10A	0.9700	O1—H1D	0.84 (2)
C10—H10B	0.9700	O2—H2C	0.88 (3)

C11—N4	1.323 (2)	O3—H3B	0.86 (3)
N1—C1—C1^{i}	110.60 (17)	C13—C12—C17	119.8 (2)
N1—C1—H1A	109.5	N4—C12—C17	109.68 (16)
C1^{i}—C1—H1A	109.5	C14—C13—C12	118.6 (2)
N1—C1—H1B	109.5	C14—C13—H13	120.7
C1^{i}—C1—H1B	109.5	C12—C13—H13	120.7
H1A—C1—H1B	108.1	C13—C14—C15	121.3 (2)
N1—C2—C3	113.09 (14)	C13—C14—H14	119.4
N1—C2—H2A	109.0	C15—C14—H14	119.4
C3—C2—H2A	109.0	C16—C15—C14	121.4 (2)
N1—C2—H2B	109.0	C16—C15—H15	119.3
C3—C2—H2B	109.0	C14—C15—H15	119.3
H2A—C2—H2B	107.8	C15—C16—C17	117.0 (2)
N2—C3—N3	113.39 (16)	C15—C16—H16	121.5
N2—C3—C2	124.18 (17)	C17—C16—H16	121.5
N3—C3—C2	122.37 (15)	N5—C17—C16	132.83 (19)
C5—C4—C9	122.96 (18)	N5—C17—C12	105.11 (17)
C5—C4—N3	131.8 (2)	C16—C17—C12	122.06 (19)
C9—C4—N3	105.17 (17)	O3—C18—H18A	109.5
C4—C5—C6	116.0 (2)	O3—C18—H18B	109.5
C4—C5—H5	122.0	H18A—C18—H18B	109.5
C6—C5—H5	122.0	O3—C18—H18C	109.5
C7—C6—C5	121.8 (2)	H18A—C18—H18C	109.5
C7—C6—H6	119.1	H18B—C18—H18C	109.5
C5—C6—H6	119.1	O2—C19—H19A	109.5
C8—C7—C6	121.9 (2)	O2—C19—H19B	109.5
C8—C7—H7	119.1	H19A—C19—H19B	109.5
C6—C7—H7	119.1	O2—C19—H19C	109.5
C7—C8—C9	117.8 (2)	H19A—C19—H19C	109.5
C7—C8—H8	121.1	H19B—C19—H19C	109.5
C9—C8—H8	121.1	C2—N1—C10	112.26 (14)
N2—C9—C4	109.66 (15)	C2—N1—C1	111.51 (13)
N2—C9—C8	130.7 (2)	C10—N1—C1	111.94 (13)
C4—C9—C8	119.6 (2)	C3—N2—C9	105.00 (16)
N1—C10—C11	110.23 (15)	C3—N3—C4	106.77 (15)
N1—C10—H10A	109.6	C3—N3—H3A	129.9 (13)
C11—C10—H10A	109.6	C4—N3—H3A	123.2 (13)
N1—C10—H10B	109.6	C11—N4—C12	104.79 (16)
C11—C10—H10B	109.6	C11—N5—C17	107.78 (16)
H10A—C10—H10B	108.1	C11—N5—H5A	121.4 (13)
N4—C11—N5	112.63 (17)	C17—N5—H5A	130.7 (13)
N4—C11—C10	125.50 (18)	H1C—O1—H1D	110 (2)
N5—C11—C10	121.80 (17)	C19—O2—H2C	109 (3)
C13—C12—N4	130.5 (2)	C18—O3—H3B	114 (4)
N1—C2—C3—N2	156.56 (17)	C13—C12—C17—C16	1.4 (3)
N1—C2—C3—N3	−26.3 (3)	N4—C12—C17—C16	−179.99 (17)
C9—C4—C5—C6	−0.1 (3)	C3—C2—N1—C10	−77.3 (2)
N3—C4—C5—C6	177.65 (19)	C3—C2—N1—C1	156.14 (16)

C4—C5—C6—C7	1.5 (3)	C11—C10—N1—C2	169.89 (14)
C5—C6—C7—C8	−1.4 (4)	C11—C10—N1—C1	−63.81 (19)
C6—C7—C8—C9	−0.3 (4)	C1^{i}—C1—N1—C2	−84.5 (2)
C5—C4—C9—N2	177.98 (17)	C1^{i}—C1—N1—C10	148.77 (19)
N3—C4—C9—N2	−0.3 (2)	N3—C3—N2—C9	0.2 (2)
C5—C4—C9—C8	−1.5 (3)	C2—C3—N2—C9	177.57 (17)
N3—C4—C9—C8	−179.79 (18)	C4—C9—N2—C3	0.0 (2)
C7—C8—C9—N2	−177.7 (2)	C8—C9—N2—C3	179.5 (2)
C7—C8—C9—C4	1.7 (3)	N2—C3—N3—C4	−0.4 (2)
N1—C10—C11—N4	132.12 (17)	C2—C3—N3—C4	−177.79 (16)
N1—C10—C11—N5	−44.6 (2)	C5—C4—N3—C3	−177.6 (2)
N4—C12—C13—C14	−179.68 (19)	C9—C4—N3—C3	0.38 (19)
C17—C12—C13—C14	−1.4 (3)	N5—C11—N4—C12	−0.37 (19)
C12—C13—C14—C15	0.8 (3)	C10—C11—N4—C12	−177.35 (15)
C13—C14—C15—C16	−0.2 (4)	C13—C12—N4—C11	178.59 (18)
C14—C15—C16—C17	0.1 (3)	C17—C12—N4—C11	0.16 (18)
C15—C16—C17—N5	179.17 (19)	N4—C11—N5—C17	0.4 (2)
C15—C16—C17—C12	−0.7 (3)	C10—C11—N5—C17	177.55 (14)
C13—C12—C17—N5	−178.53 (16)	C16—C17—N5—C11	179.8 (2)
N4—C12—C17—N5	0.09 (19)	C12—C17—N5—C11	−0.30 (18)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1C···O2	0.87 (2)	1.85 (2)	2.702 (3)	164 (3)
O3—H3B···N2^{ii}	0.86 (3)	1.90 (4)	2.731 (2)	163 (5)
N5—H5A···O1^{iii}	0.895 (19)	1.94 (2)	2.828 (2)	169.5 (19)
N3—H3A···O1^{iii}	0.899 (18)	1.972 (19)	2.862 (2)	170.0 (18)
O2—H2C···N4^{iv}	0.88 (3)	1.89 (3)	2.765 (3)	173 (5)
O1—H1D···O3^{v}	0.84 (2)	1.89 (2)	2.731 (3)	177 (3)

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

Fig. 1

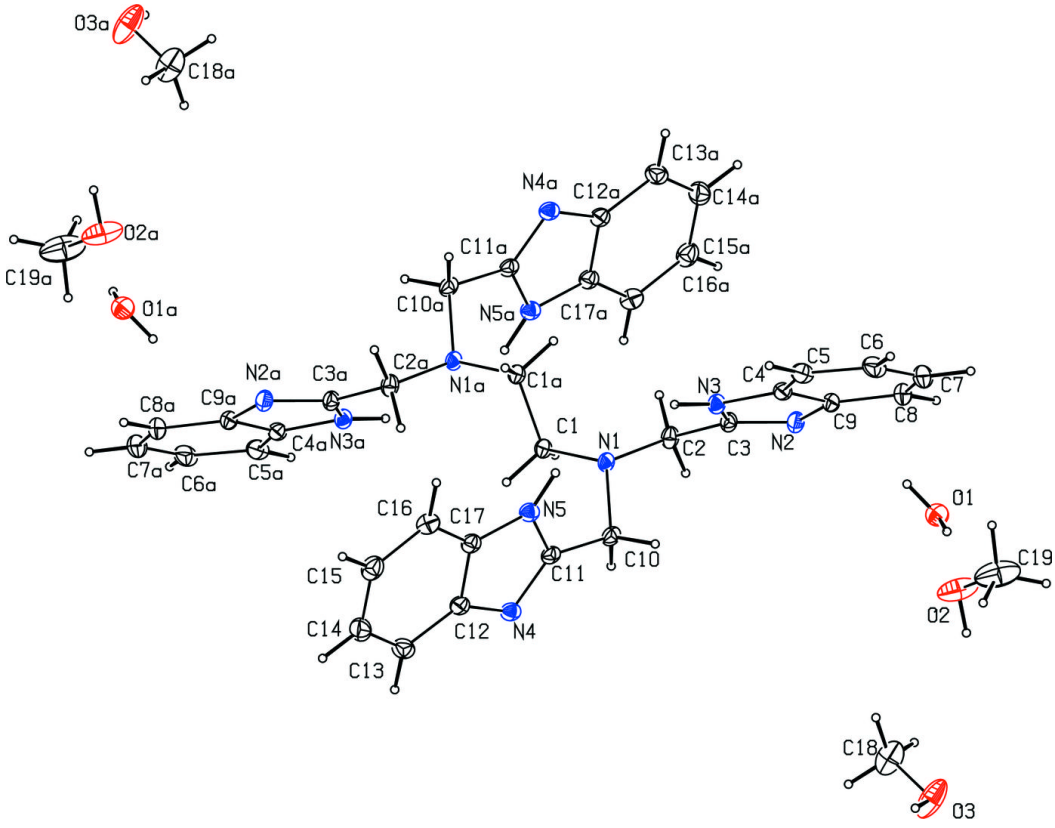
O3a
C18a
C13a
N4a
C12a
C14a
O2a
C19a
C11a
C15a
O1a
C10a
N5a
C17a
C16a
N2a
C3a
C2a
N1a
C1a
C5
C6
C4
N3
C7
C8a
C9a
C1
N1
C9
C8
C4a
N3a
C2
C3
N2
C7a
C6a
C5a
C16
C17
N5
O1
C15
C11
C10
C19
C14
C12
N4
O2
C13
C18
O3

Fig. 2