IUCrData

ISSN 2414-3146

1,1′-Methylenebis(4-*tert*-butylpyridinium) dichloride hemihydrate

J.P.J. Bruekers, J.A.A.W. Elemans, R.J.M. Nolte and P. Tinnemans*

Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ, Nijmegen, The Netherlands. *Correspondence e-mail: p.tinnemans@science.ru.nl

Received 19 July 2021
Accepted 27 July 2021

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

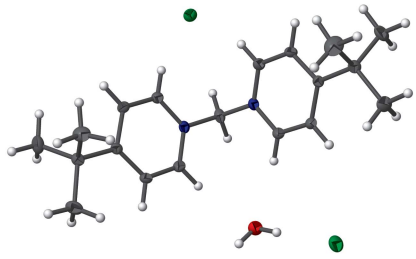
Keywords: crystal structure; O—H···Cl hydrogen bonds; Cl···π contacts.

CCDC reference: 2099687

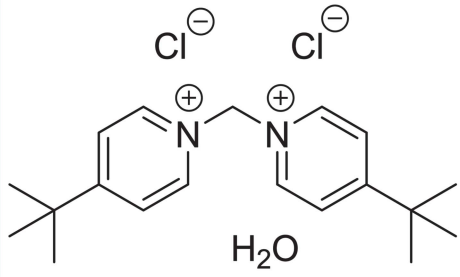
Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title hydrated salt, $C_{19}H_{28}N_2^{2+}\cdot 2Cl^-\cdot 0.5H_2O$, at 150 K has monoclinic (*C*2/*c*) symmetry. The water molecule is located on a twofold rotation axis.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) was prepared before by mixing 4-*tert*-butylpyridine with dichloromethane in DMSO (Rudine *et al.*, 2010). The crystal structure of a related compound, 1,1′-methylenebis(4-*tert*-butylpyridinium)chloridocobaltate(II)–dichloromethane (1:1), has been determined (Ayom *et al.*, 2019). The di-cation of the title compound has a V-shaped structure caused by the bridging methylene group with an N—C—N angle of 109.30 (10)°. One of the chloride anions forms a hydrogen bond with the water molecule (Table 1). The other chloride anion is clamped between the aromatic rings (Fig. 2) by electrostatic and anion–π interactions with distances to the centroid of the mean planes through the pyridinium rings of 3.3907 (6) and 3.4135 (6) Å, which are similar to the distances of anion–π interactions in the literature (Kan *et al.*, 2018; Demeshko *et al.*, 2004).

Synthesis and crystallization

The title compound was obtained during an attempt to grow single crystals of 4-*tert*-butylpyridine coordinated to a cadmium derivative of a porphyrin diphenylglycoluril cage reported by Gilissen *et al.* (2019) by slow evaporation from a 4-*tert*-butylpyridine/dichloromethane/heptane (1:2:2, *v*/*v*/*v*) mixture. The mixture was left at 298 K. Colorless needle-shaped crystals were obtained after one week.

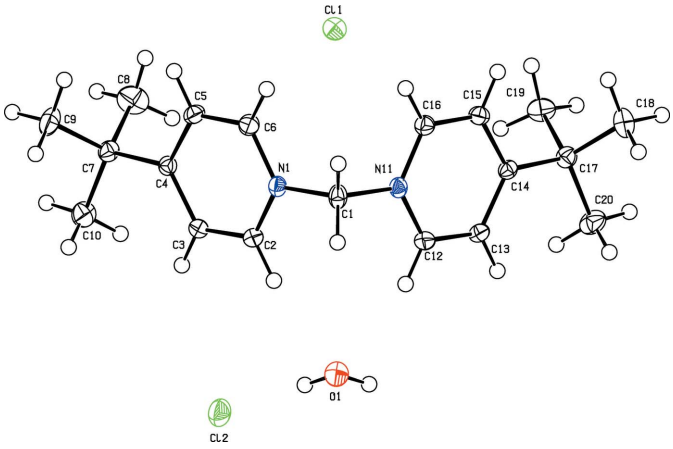


Figure 1
Molecular structure of the title compound with atom labels. Displacement ellipsoids are at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

Funding for this research was provided by: European Research Council (grant No. 74092, ERC Advanced to R. J. M. Nolte); Dutch Ministry of Education, Culture, and Science (grant No. 024.001.035, Gravitation program).

References

Ayom, G. E., Zamisa, S. J. & Van Zyl, W. E. (2019). *Z. Kristallogr. New Cryst. Struct.* **234**, 629–631.

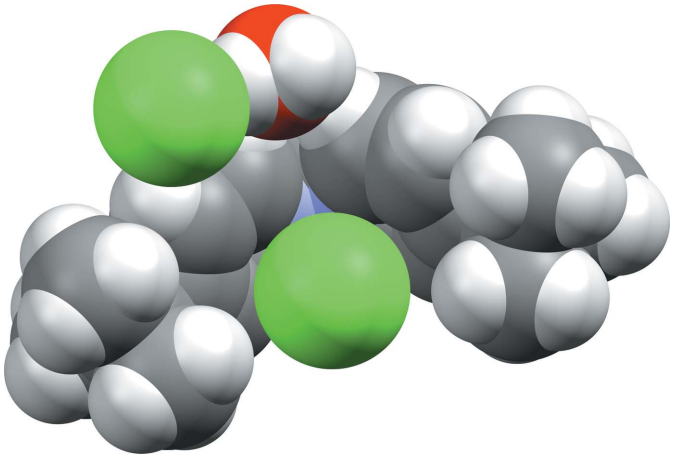


Figure 2
Space-filling representation of the title compound showing one chloride hydrogen bonded to the water molecule and a chloride ion clamped between the aromatic rings.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Cl2^{i}	0.829 (19)	2.223 (19)	3.0513 (10)	179 (2)

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{28}N_2^{2+}\cdot 2Cl^-\cdot 0.5H_2O$
M_r	364.34
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	27.7659 (8), 5.9001 (2), 23.9758 (7)
β (°)	97.4152 (14)
V (Å^3)	3894.9 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.34
Crystal size (mm)	0.55 × 0.14 × 0.03
Data collection	
Diffractometer	Bruker D8 Quest APEX3
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.601, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36472, 7428, 5988
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.106, 1.09
No. of reflections	7428
No. of parameters	222
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.34

Computer programs: *APEX3* (Bruker, 2017), *SAINT* (Bruker, 2003), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020) and *shelXle* (Hübschle *et al.*, 2011).

Bruker (2003). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2017). *APEX3*. Bruker AXS Inc., Madison, Wisconsin, USA.
Demeshko, S., Dechert, S. & Meyer, F. (2004). *J. Am. Chem. Soc.* **126**, 4508–4509.
Gilissen, P. J., Swartjes, A., Spierenburg, B., Bruekers, J. P. J., Tinnemans, P., White, P. B., Rutjes, F. P. J. T., Nolte, R. J. M. & Elemans, J. A. A. W. (2019). *Tetrahedron*, **75**, 4640–4647.
Hübschle, C. B., Sheldrick, G. M. & Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281–1284.
Kan, X., Liu, H., Pan, Q., Li, Z. & Zhao, Y. (2018). *Chin. Chem. Lett.* **29**, 261–266.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Rudine, A. B., Walter, M. G. & Wamser, C. C. (2010). *J. Org. Chem.* **75**, 4292–4295.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

full crystallographic data

IUCrData (2021). **6**, x210768 [https://doi.org/10.1107/S2414314621007689]

1,1′-Methylenebis(4-*tert*-butylpyridinium) dichloride hemihydrate

J.P.J. Bruekers, J.A.A.W. Elemans, R.J.M. Nolte and P. Tinnemans

1,1′-Methylenebis(4-*tert*-butylpyridinium) dichloride hemihydrate

Crystal data

$C_{19}H_{28}N_2^{2+}\cdot 2Cl^-\cdot 0.5H_2O$
$M_r = 364.34$
Monoclinic, $C2/c$
$a = 27.7659\ (8)$ Å
$b = 5.9001\ (2)$ Å
$c = 23.9758\ (7)$ Å
$\beta = 97.4152\ (14)°$
$V = 3894.9\ (2)$ Å^3
$Z = 8$
$F(000) = 1560$
$D_x = 1.243$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9986 reflections
$\theta = 2.4–32.9°$
$\mu = 0.34$ mm^{-1}
$T = 150$ K
Needle, colourless
0.55 × 0.14 × 0.03 mm

Data collection

Bruker D8 Quest APEX3 diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 7.41 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.601$, $T_{max} = 0.747$
36472 measured reflections
7428 independent reflections
5988 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 33.2°$, $\theta_{min} = 2.4°$
$h = -40\rightarrow 42$
$k = -9\rightarrow 7$
$l = -36\rightarrow 36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.106$
$S = 1.09$
7428 reflections
222 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 4.7462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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. Non-hydrogen atoms were refined freely with anisotropic displacement parameters. Hydrogen atoms were placed on calculated positions or located in difference Fourier maps. Hydrogen atoms bonded to C were refined with a riding model with U(H)= 1.2U_{eq}($C_{aromatic}$) or U(H)= 1.5U_{eq}(C_{methyl}). The coordinates of the H atom bonded to O were refined with U(H)= 1.5U_{eq}(O).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.66762 (2)	1.24711 (5)	0.69007 (2)	0.02011 (7)
Cl2	0.46510 (2)	−0.04518 (7)	0.65504 (2)	0.02807 (9)
O1	0.500000	0.2834 (2)	0.750000	0.0226 (3)
H1	0.5097 (7)	0.194 (3)	0.7757 (8)	0.034*
N1	0.58269 (4)	0.70318 (18)	0.66729 (4)	0.01528 (19)
C1	0.58379 (5)	0.8164 (2)	0.72238 (5)	0.0183 (2)
H1A	0.594236	0.975901	0.719446	0.022*
H1B	0.550893	0.815733	0.734115	0.022*
C2	0.55369 (5)	0.5221 (2)	0.65514 (5)	0.0184 (2)
H2	0.533083	0.472634	0.681422	0.022*
C3	0.55359 (5)	0.4077 (2)	0.60496 (5)	0.0178 (2)
H3	0.532917	0.280414	0.596878	0.021*
C4	0.58376 (4)	0.4784 (2)	0.56596 (5)	0.0147 (2)
C5	0.61278 (5)	0.6685 (2)	0.58025 (5)	0.0185 (2)
H5	0.633346	0.723036	0.554488	0.022*
C6	0.61224 (5)	0.7782 (2)	0.63070 (5)	0.0183 (2)
H6	0.632542	0.906011	0.639799	0.022*
C7	0.58699 (5)	0.3558 (2)	0.51056 (5)	0.0178 (2)
C8	0.63866 (6)	0.2601 (3)	0.51317 (8)	0.0325 (3)
H8A	0.641469	0.173104	0.478916	0.049*
H8B	0.645413	0.160829	0.546031	0.049*
H8C	0.662081	0.385129	0.516240	0.049*
C9	0.57717 (6)	0.5233 (3)	0.46124 (6)	0.0272 (3)
H9A	0.579490	0.443658	0.425820	0.041*
H9B	0.601237	0.645579	0.465983	0.041*
H9C	0.544529	0.587349	0.460507	0.041*
C10	0.55031 (6)	0.1622 (3)	0.50068 (6)	0.0261 (3)
H10A	0.517323	0.222912	0.499241	0.039*
H10B	0.556244	0.052461	0.531479	0.039*
H10C	0.553860	0.087118	0.464978	0.039*
N11	0.61792 (4)	0.69581 (19)	0.76441 (4)	0.01542 (19)
C12	0.60175 (5)	0.5233 (2)	0.79374 (5)	0.0185 (2)
H12	0.568214	0.485537	0.788490	0.022*
C13	0.63333 (5)	0.4013 (2)	0.83121 (5)	0.0178 (2)
H13	0.621456	0.280122	0.851674	0.021*
C14	0.68271 (4)	0.4544 (2)	0.83935 (5)	0.0149 (2)
C15	0.69812 (4)	0.6362 (2)	0.80819 (5)	0.0169 (2)
H15	0.731437	0.678077	0.812838	0.020*
C16	0.66551 (5)	0.7540 (2)	0.77110 (5)	0.0173 (2)
H16	0.676331	0.876209	0.750120	0.021*

C17	0.71984 (5)	0.3212 (2)	0.87856 (5)	0.0179 (2)
C18	0.74794 (6)	0.4840 (3)	0.92118 (6)	0.0267 (3)
H18A	0.764762	0.597771	0.901042	0.040*
H18B	0.771764	0.398124	0.946550	0.040*
H18C	0.725171	0.559656	0.943085	0.040*
C19	0.75542 (5)	0.2126 (2)	0.84213 (6)	0.0245 (3)
H19A	0.737128	0.126977	0.811366	0.037*
H19B	0.777406	0.110051	0.865328	0.037*
H19C	0.774353	0.331603	0.826525	0.037*
C20	0.69621 (5)	0.1354 (3)	0.91046 (6)	0.0262 (3)
H20A	0.678134	0.031685	0.883493	0.039*
H20B	0.673927	0.204551	0.934073	0.039*
H20C	0.721457	0.051023	0.934211	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02257 (14)	0.01460 (13)	0.02306 (14)	−0.00075 (11)	0.00262 (10)	−0.00094 (11)
Cl2	0.03340 (18)	0.03155 (18)	0.01914 (14)	−0.00159 (15)	0.00295 (12)	−0.00336 (13)
O1	0.0265 (7)	0.0178 (7)	0.0234 (7)	0.000	0.0025 (5)	0.000
N1	0.0157 (4)	0.0171 (5)	0.0130 (4)	0.0015 (4)	0.0012 (3)	−0.0009 (3)
C1	0.0191 (5)	0.0215 (6)	0.0139 (5)	0.0059 (5)	0.0006 (4)	−0.0027 (4)
C2	0.0163 (5)	0.0236 (6)	0.0159 (5)	−0.0028 (5)	0.0035 (4)	0.0004 (4)
C3	0.0168 (5)	0.0202 (6)	0.0161 (5)	−0.0044 (5)	0.0012 (4)	0.0002 (4)
C4	0.0148 (5)	0.0153 (5)	0.0139 (5)	0.0010 (4)	0.0011 (4)	0.0011 (4)
C5	0.0212 (6)	0.0192 (6)	0.0160 (5)	−0.0053 (5)	0.0055 (4)	−0.0002 (4)
C6	0.0217 (6)	0.0161 (6)	0.0170 (5)	−0.0033 (5)	0.0019 (4)	−0.0003 (4)
C7	0.0203 (6)	0.0171 (6)	0.0165 (5)	−0.0002 (5)	0.0044 (4)	−0.0023 (4)
C8	0.0264 (7)	0.0316 (8)	0.0410 (8)	0.0069 (6)	0.0094 (6)	−0.0095 (7)
C9	0.0396 (8)	0.0274 (7)	0.0148 (5)	−0.0023 (6)	0.0043 (5)	0.0002 (5)
C10	0.0337 (7)	0.0226 (7)	0.0222 (6)	−0.0074 (6)	0.0045 (5)	−0.0071 (5)
N11	0.0156 (4)	0.0179 (5)	0.0128 (4)	0.0015 (4)	0.0017 (3)	−0.0020 (4)
C12	0.0150 (5)	0.0236 (6)	0.0173 (5)	−0.0023 (5)	0.0039 (4)	−0.0005 (5)
C13	0.0184 (5)	0.0196 (6)	0.0159 (5)	−0.0031 (5)	0.0047 (4)	0.0016 (4)
C14	0.0168 (5)	0.0148 (5)	0.0136 (5)	0.0000 (4)	0.0039 (4)	−0.0013 (4)
C15	0.0151 (5)	0.0174 (6)	0.0183 (5)	−0.0019 (4)	0.0026 (4)	−0.0004 (4)
C16	0.0186 (5)	0.0173 (5)	0.0162 (5)	−0.0025 (5)	0.0026 (4)	−0.0002 (4)
C17	0.0188 (5)	0.0171 (5)	0.0178 (5)	0.0019 (4)	0.0024 (4)	0.0018 (4)
C18	0.0298 (7)	0.0269 (7)	0.0212 (6)	0.0023 (6)	−0.0051 (5)	−0.0021 (5)
C19	0.0223 (6)	0.0213 (7)	0.0313 (7)	0.0042 (5)	0.0087 (5)	−0.0002 (5)
C20	0.0272 (7)	0.0249 (7)	0.0273 (7)	0.0038 (6)	0.0065 (5)	0.0108 (6)

Geometric parameters (Å, º)

O1—H1	0.829 (19)	C10—H10A	0.9800
O1—H1^{i}	0.829 (19)	C10—H10B	0.9800
N1—C2	1.3468 (17)	C10—H10C	0.9800
N1—C6	1.3509 (16)	N11—C12	1.3465 (17)

N1—C1	1.4768 (16)	N11—C16	1.3547 (16)
C1—N11	1.4740 (16)	C12—C13	1.3749 (18)
C1—H1A	0.9900	C12—H12	0.9500
C1—H1B	0.9900	C13—C14	1.3955 (17)
C2—C3	1.3792 (18)	C13—H13	0.9500
C2—H2	0.9500	C14—C15	1.4048 (17)
C3—C4	1.3972 (17)	C14—C17	1.5213 (18)
C3—H3	0.9500	C15—C16	1.3732 (18)
C4—C5	1.3976 (18)	C15—H15	0.9500
C4—C7	1.5249 (17)	C16—H16	0.9500
C5—C6	1.3735 (18)	C17—C20	1.5320 (19)
C5—H5	0.9500	C17—C18	1.539 (2)
C6—H6	0.9500	C17—C19	1.5402 (19)
C7—C10	1.528 (2)	C18—H18A	0.9800
C7—C8	1.536 (2)	C18—H18B	0.9800
C7—C9	1.5379 (19)	C18—H18C	0.9800
C8—H8A	0.9800	C19—H19A	0.9800
C8—H8B	0.9800	C19—H19B	0.9800
C8—H8C	0.9800	C19—H19C	0.9800
C9—H9A	0.9800	C20—H20A	0.9800
C9—H9B	0.9800	C20—H20B	0.9800
C9—H9C	0.9800	C20—H20C	0.9800

H1—O1—H1^{i}	101 (3)	C7—C10—H10C	109.5
C2—N1—C6	121.04 (11)	H10A—C10—H10C	109.5
C2—N1—C1	119.67 (11)	H10B—C10—H10C	109.5
C6—N1—C1	119.24 (11)	C12—N11—C16	121.02 (11)
N11—C1—N1	109.30 (10)	C12—N11—C1	119.58 (11)
N11—C1—H1A	109.8	C16—N11—C1	119.33 (11)
N1—C1—H1A	109.8	N11—C12—C13	120.63 (11)
N11—C1—H1B	109.8	N11—C12—H12	119.7
N1—C1—H1B	109.8	C13—C12—H12	119.7
H1A—C1—H1B	108.3	C12—C13—C14	120.39 (12)
N1—C2—C3	120.71 (11)	C12—C13—H13	119.8
N1—C2—H2	119.6	C14—C13—H13	119.8
C3—C2—H2	119.6	C13—C14—C15	117.28 (11)
C2—C3—C4	120.27 (12)	C13—C14—C17	123.06 (11)
C2—C3—H3	119.9	C15—C14—C17	119.63 (11)
C4—C3—H3	119.9	C16—C15—C14	120.66 (11)
C3—C4—C5	116.85 (11)	C16—C15—H15	119.7
C3—C4—C7	123.32 (11)	C14—C15—H15	119.7
C5—C4—C7	119.82 (11)	N11—C16—C15	120.01 (12)
C6—C5—C4	121.52 (11)	N11—C16—H16	120.0
C6—C5—H5	119.2	C15—C16—H16	120.0
C4—C5—H5	119.2	C14—C17—C20	112.25 (11)
N1—C6—C5	119.61 (12)	C14—C17—C18	109.44 (11)
N1—C6—H6	120.2	C20—C17—C18	109.15 (11)
C5—C6—H6	120.2	C14—C17—C19	107.32 (10)

C4—C7—C10	112.12 (10)	C20—C17—C19	109.42 (12)
C4—C7—C8	107.37 (11)	C18—C17—C19	109.20 (12)
C10—C7—C8	109.36 (12)	C17—C18—H18A	109.5
C4—C7—C9	109.91 (11)	C17—C18—H18B	109.5
C10—C7—C9	108.22 (12)	H18A—C18—H18B	109.5
C8—C7—C9	109.86 (12)	C17—C18—H18C	109.5
C7—C8—H8A	109.5	H18A—C18—H18C	109.5
C7—C8—H8B	109.5	H18B—C18—H18C	109.5
H8A—C8—H8B	109.5	C17—C19—H19A	109.5
C7—C8—H8C	109.5	C17—C19—H19B	109.5
H8A—C8—H8C	109.5	H19A—C19—H19B	109.5
H8B—C8—H8C	109.5	C17—C19—H19C	109.5
C7—C9—H9A	109.5	H19A—C19—H19C	109.5
C7—C9—H9B	109.5	H19B—C19—H19C	109.5
H9A—C9—H9B	109.5	C17—C20—H20A	109.5
C7—C9—H9C	109.5	C17—C20—H20B	109.5
H9A—C9—H9C	109.5	H20A—C20—H20B	109.5
H9B—C9—H9C	109.5	C17—C20—H20C	109.5
C7—C10—H10A	109.5	H20A—C20—H20C	109.5
C7—C10—H10B	109.5	H20B—C20—H20C	109.5
H10A—C10—H10B	109.5		

C2—N1—C1—N11	84.05 (14)	N1—C1—N11—C12	−89.45 (13)
C6—N1—C1—N11	−93.47 (14)	N1—C1—N11—C16	87.62 (14)
C6—N1—C2—C3	0.26 (19)	C16—N11—C12—C13	−0.16 (19)
C1—N1—C2—C3	−177.21 (12)	C1—N11—C12—C13	176.86 (11)
N1—C2—C3—C4	0.1 (2)	N11—C12—C13—C14	−0.08 (19)
C2—C3—C4—C5	−0.76 (19)	C12—C13—C14—C15	0.39 (18)
C2—C3—C4—C7	177.78 (12)	C12—C13—C14—C17	−177.78 (12)
C3—C4—C5—C6	1.09 (19)	C13—C14—C15—C16	−0.48 (18)
C7—C4—C5—C6	−177.51 (12)	C17—C14—C15—C16	177.75 (12)
C2—N1—C6—C5	0.06 (19)	C12—N11—C16—C15	0.07 (18)
C1—N1—C6—C5	177.54 (12)	C1—N11—C16—C15	−176.96 (11)
C4—C5—C6—N1	−0.8 (2)	C14—C15—C16—N11	0.26 (19)
C3—C4—C7—C10	5.16 (18)	C13—C14—C17—C20	−3.89 (17)
C5—C4—C7—C10	−176.34 (12)	C15—C14—C17—C20	177.98 (12)
C3—C4—C7—C8	−114.97 (14)	C13—C14—C17—C18	−125.25 (13)
C5—C4—C7—C8	63.53 (16)	C15—C14—C17—C18	56.62 (15)
C3—C4—C7—C9	125.57 (13)	C13—C14—C17—C19	116.37 (13)
C5—C4—C7—C9	−55.93 (16)	C15—C14—C17—C19	−61.76 (15)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···Cl2^{i}	0.829 (19)	2.223 (19)	3.0513 (10)	179 (2)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.