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Crystal structure of 2-cyano-1-methylpyridinium perchlorate

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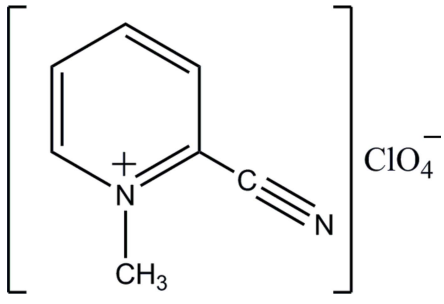
The asymmetric unit of the title salt, $C_7H_7N_2^+\cdot ClO_4^-$, comprises two independent formula units. The solid-state structure comprises corrugated layers of cations and of anions, approximately parallel to (010). The supramolecular layers are stabilized and connected by C—H···O hydrogen bonding to consolidate a three-dimensional architecture. A close pyridinium–perchlorate N···O contact [2.867 (5) Å] is noted. The crystal was refined as an inversion twin.

Keywords: crystal structure; salt; pyridinium; perchlorate; hydrogen bonding.

CCDC reference: 1430590

1. Related literature

For structures of other salts of the 2-cyano-1-methylpyridinium cation, see: Koplitz *et al.* (2012); Kammer *et al.* (2013); Vaccaro *et al.* (2015). For structures of salts of the isomeric 2-cyanoanilinium cation, see: Zhang (2009); Cui & Chen (2010).



2. Experimental

2.1. Crystal data

$C_7H_7N_2^+\cdot ClO_4^-$
M_r = 218.60
Monoclinic, $P2_1$
a = 8.0112 (12) Å
b = 7.7011 (12) Å
c = 14.742 (2) Å
β = 90.982 (2)°
V = 909.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 150 K
0.19 × 0.14 × 0.13 mm

2.2. Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.93, T_{max} = 0.95
22843 measured reflections
22843 independent reflections
20913 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
S = 1.00
22843 reflections
256 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack x determined using 1908 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.04 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O1^{i}	0.98	2.53	3.441 (5)	154
C1—H1C···O3	0.98	2.52	3.164 (5)	123
C3—H3···O5^{ii}	0.95	2.54	3.326 (5)	140
C5—H5···O8^{iii}	0.95	2.66	3.262 (6)	122
C6—H6···O1^{i}	0.95	2.55	3.415 (6)	152
C6—H6···O4^{i}	0.95	2.65	3.534 (6)	155
C8—H8A···O1^{iv}	0.98	2.55	3.294 (6)	132
C8—H8B···O7^{v}	0.98	2.57	3.538 (6)	169
C8—H8C···O6	0.98	2.51	3.425 (5)	156
C10—H10···O2^{vi}	0.95	2.51	3.367 (5)	150
C12—H12···O2^{vii}	0.95	2.52	3.347 (5)	145
C13—H13···O6	0.95	2.35	3.247 (6)	156

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* and *CELL_NOW* (Sheldrick, 2008*a*); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008*b*).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5395).

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supporting information

Acta Cryst. (2015). E**71**, o852–o853 [doi:10.1107/S2056989015019155]

Crystal structure of 2-cyano-1-methylpyridinium perchlorate

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S1. Comment

The asymmetric unit comprises two independent formula units. A portion of the C—H···O hydrogen bonding network which aids the packing of the several ions is shown in Fig. 1 with a fuller depiction appearing in Figs 2 and 3. The solid state structure consists of corrugated layers of cations and anions formed by C—H···O hydrogen bonding between them and approximately parallel to (010). These layers are held to one another by additional C—H···O interactions. The overall structure is essentially the same as found for the tetrafluoroborate salt (Vaccaro *et al.*, 2015).

S2. Experimental

2-Cyano-1-methylpyridinium iodide (0.42 g, 1.70 mmol; m.p. 146–150°) was dissolved in a solution of silver perchlorate previously prepared by reacting Ag_2O (0.20 g, 0.86 mmol) with 1*M* aqueous $HClO_4$ (1.8 ml) in 8.0 ml of H_2O. After stirring, the precipitated AgI was removed by vacuum filtration. The filtrate was slowly evaporated to dryness in a freezer at about -5° over several months to form crystals suitable for single-crystal X-ray diffraction.

S3. Refinement

H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. The crystal was refined as a 2-component twin.

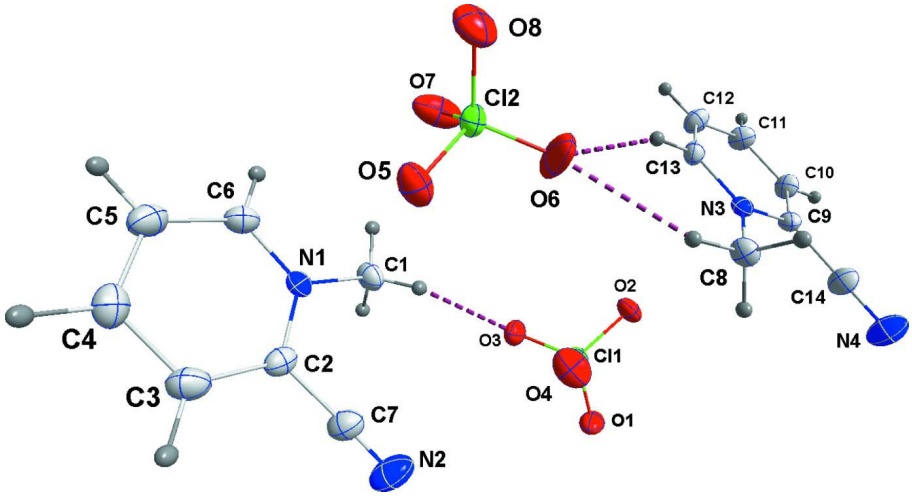

Figure 1

Perspective view of the asymmetric unit with 50% probability ellipsoids. C—H···O interactions are shown by dotted lines.

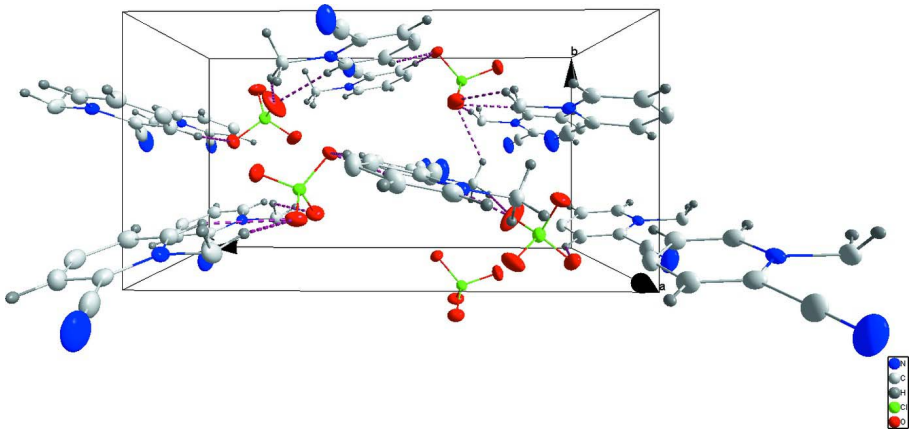

Figure 2

Packing viewed down the *a* axis showing an edge view of two corrugated layers and the C—H···O interaction (dotted line) holding them together.

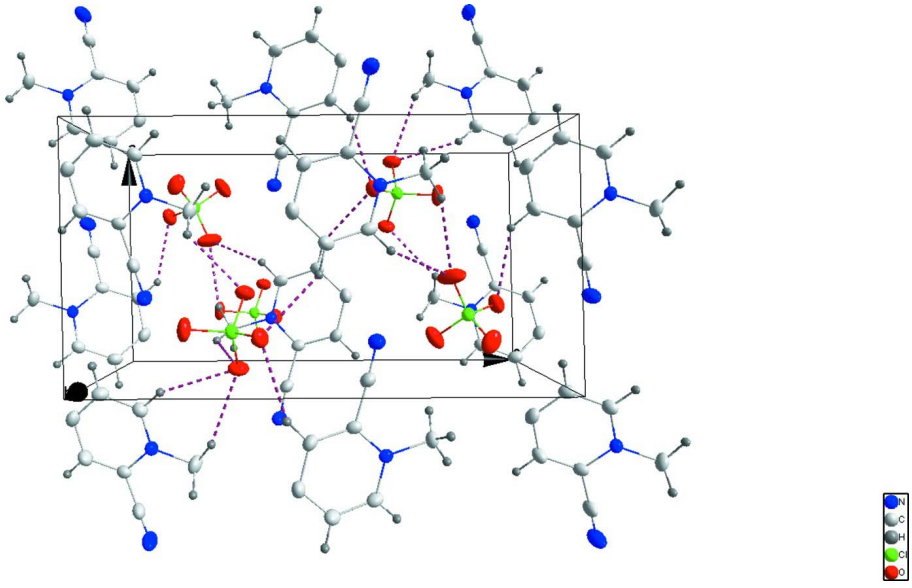

Figure 3

Packing viewed down the *b* axis providing a plan view of the corrugated sheets with C—H···O interactions shown as dotted lines.

2-Cyano-1-methylpyridinium perchlorate

Crystal data

$C_7H_7N_2^+·ClO_4^-$
M_r = 218.60
Monoclinic, $P2_1$
a = 8.0112 (12) Å
b = 7.7011 (12) Å
c = 14.742 (2) Å
β = 90.982 (2)°
V = 909.4 (2) Å^3
Z = 4
$F(000)$ = 448
D_x = 1.597 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9987 reflections
θ = 2.5–29.2°
μ = 0.41 mm^{-1}
T = 150 K
Block, colourless
0.19 × 0.14 × 0.13 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3660 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.93, T_{max} = 0.95
22843 measured reflections
22843 independent reflections
20913 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 29.2°, θ_{min} = 2.5°
h = −10→10
k = −10→10
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
S = 1.00
22843 reflections
256 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack x determined using 1908 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.04 (3)

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, collected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = -30.00 and 210.00°. The scan time was 15 sec/frame. Analysis of 3152 reflections having I/σ(I) > 13 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008a) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about c*. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.2547 (4)	0.1723 (5)	0.8742 (2)	0.0186 (7)
N2	0.6652 (5)	0.0531 (8)	0.8975 (3)	0.0424 (14)
C1	0.3149 (5)	0.1871 (7)	0.7797 (3)	0.0268 (10)
H1A	0.2255	0.2339	0.7406	0.040*
H1B	0.3474	0.0721	0.7577	0.040*
H1C	0.4115	0.2651	0.7785	0.040*
C2	0.3617 (5)	0.1208 (6)	0.9418 (3)	0.0204 (10)

C3	0.3089 (5)	0.1017 (7)	1.0292 (3)	0.0262 (11)
H3	0.3845	0.0658	1.0759	0.031*
C4	0.1425 (5)	0.1359 (7)	1.0482 (3)	0.0261 (11)
H4	0.1033	0.1237	1.1083	0.031*
C5	0.0358 (5)	0.1874 (7)	0.9798 (3)	0.0265 (11)
H5	−0.0780	0.2106	0.9921	0.032*
C6	0.0947 (5)	0.2053 (7)	0.8927 (3)	0.0237 (10)
H6	0.0208	0.2414	0.8453	0.028*
C7	0.5316 (5)	0.0839 (8)	0.9162 (3)	0.0266 (11)
Cl1	0.77813 (11)	0.34996 (12)	0.68489 (7)	0.0185 (2)
O1	0.9290 (4)	0.2488 (5)	0.6789 (3)	0.0300 (8)
O2	0.7857 (4)	0.4925 (4)	0.6214 (2)	0.0263 (7)
O3	0.6375 (4)	0.2420 (5)	0.6622 (3)	0.0295 (9)
O4	0.7628 (4)	0.4142 (5)	0.7754 (2)	0.0370 (9)
N3	0.7638 (4)	0.8780 (5)	0.6208 (3)	0.0167 (8)
N4	1.1905 (4)	0.9228 (7)	0.6055 (3)	0.0374 (12)
C8	0.8152 (5)	0.8446 (7)	0.7165 (3)	0.0214 (9)
H8A	0.8523	0.9534	0.7448	0.032*
H8B	0.9070	0.7604	0.7181	0.032*
H8C	0.7203	0.7979	0.7497	0.032*
C9	0.8788 (4)	0.9197 (6)	0.5573 (3)	0.0187 (9)
C10	0.8332 (5)	0.9575 (7)	0.4697 (3)	0.0232 (10)
H10	0.9152	0.9855	0.4263	0.028*
C11	0.6647 (5)	0.9542 (7)	0.4452 (3)	0.0254 (10)
H11	0.6295	0.9816	0.3850	0.030*
C12	0.5499 (5)	0.9103 (7)	0.5099 (4)	0.0253 (11)
H12	0.4345	0.9046	0.4942	0.030*
C13	0.6021 (4)	0.8747 (6)	0.5969 (3)	0.0214 (10)
H13	0.5216	0.8472	0.6413	0.026*
C14	1.0526 (5)	0.9217 (7)	0.5867 (4)	0.0259 (11)
Cl2	0.26845 (11)	0.66595 (14)	0.81449 (7)	0.0213 (2)
O5	0.3040 (4)	0.5521 (5)	0.8898 (2)	0.0329 (9)
O6	0.4209 (4)	0.7202 (7)	0.7750 (3)	0.0629 (16)
O7	0.1683 (5)	0.5742 (6)	0.7490 (3)	0.0436 (10)
O8	0.1756 (4)	0.8134 (5)	0.8449 (3)	0.0405 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0224 (14)	0.0147 (18)	0.0187 (19)	−0.0010 (15)	0.0002 (13)	0.0016 (17)
N2	0.0285 (19)	0.069 (4)	0.030 (3)	0.009 (2)	−0.0004 (17)	−0.009 (3)
C1	0.034 (2)	0.026 (3)	0.020 (2)	0.004 (2)	0.0063 (17)	0.004 (2)
C2	0.0181 (16)	0.018 (3)	0.025 (3)	−0.0009 (15)	−0.0016 (15)	−0.003 (2)
C3	0.026 (2)	0.030 (3)	0.023 (3)	0.0038 (19)	−0.0050 (17)	−0.001 (2)
C4	0.0295 (19)	0.028 (3)	0.021 (2)	−0.0039 (18)	0.0058 (16)	−0.001 (2)
C5	0.0207 (18)	0.027 (3)	0.032 (3)	0.0011 (19)	0.0009 (16)	0.000 (2)
C6	0.0229 (18)	0.023 (3)	0.025 (3)	0.0020 (17)	−0.0027 (16)	−0.001 (2)
C7	0.026 (2)	0.035 (3)	0.019 (3)	0.003 (2)	−0.0029 (17)	−0.004 (2)

Cl1	0.0208 (4)	0.0165 (5)	0.0182 (5)	0.0004 (4)	−0.0004 (3)	−0.0003 (4)
O1	0.0220 (14)	0.0215 (19)	0.046 (2)	0.0039 (12)	−0.0011 (14)	0.0018 (18)
O2	0.0350 (15)	0.0197 (18)	0.0240 (18)	−0.0006 (13)	−0.0028 (13)	0.0059 (15)
O3	0.0232 (14)	0.026 (2)	0.040 (2)	−0.0055 (13)	−0.0023 (13)	0.0019 (17)
O4	0.056 (2)	0.035 (2)	0.0192 (17)	0.0011 (18)	0.0047 (16)	−0.0051 (16)
N3	0.0189 (14)	0.0122 (19)	0.019 (2)	0.0020 (13)	0.0013 (13)	−0.0005 (15)
N4	0.0229 (17)	0.061 (4)	0.028 (2)	0.0016 (19)	0.0012 (16)	0.003 (2)
C8	0.0263 (17)	0.022 (2)	0.016 (2)	−0.0008 (19)	−0.0004 (15)	0.001 (2)
C9	0.0162 (16)	0.016 (2)	0.024 (2)	0.0016 (15)	0.0018 (15)	0.000 (2)
C10	0.0225 (18)	0.027 (3)	0.020 (2)	−0.0014 (17)	0.0054 (16)	−0.001 (2)
C11	0.0272 (19)	0.031 (3)	0.017 (2)	0.0028 (19)	−0.0008 (17)	−0.001 (2)
C12	0.0205 (17)	0.031 (3)	0.025 (3)	−0.0007 (17)	−0.0022 (17)	−0.006 (2)
C13	0.0180 (16)	0.019 (3)	0.027 (3)	−0.0033 (16)	0.0034 (15)	−0.004 (2)
C14	0.0213 (19)	0.033 (3)	0.024 (3)	0.0006 (18)	0.0052 (17)	0.000 (2)
Cl2	0.0207 (4)	0.0245 (6)	0.0188 (5)	−0.0032 (4)	0.0023 (3)	0.0007 (5)
O5	0.0409 (18)	0.032 (2)	0.026 (2)	−0.0075 (16)	−0.0042 (15)	0.0064 (17)
O6	0.0260 (17)	0.092 (4)	0.071 (3)	−0.0020 (19)	0.0140 (17)	0.046 (3)
O7	0.058 (2)	0.030 (2)	0.042 (2)	0.0098 (18)	−0.0241 (18)	−0.011 (2)
O8	0.058 (2)	0.021 (2)	0.043 (2)	0.0024 (17)	0.0123 (18)	−0.0073 (18)

Geometric parameters (Å, º)

N1—C6	1.338 (5)	N3—C13	1.337 (5)
N1—C2	1.363 (6)	N3—C9	1.363 (5)
N1—C1	1.487 (5)	N3—C8	1.486 (6)
N2—C7	1.135 (6)	N4—C14	1.134 (5)
C1—H1A	0.9800	C8—H8A	0.9800
C1—H1B	0.9800	C8—H8B	0.9800
C1—H1C	0.9800	C8—H8C	0.9800
C2—C3	1.370 (6)	C9—C10	1.368 (6)
C2—C7	1.446 (6)	C9—C14	1.451 (5)
C3—C4	1.392 (6)	C10—C11	1.391 (5)
C3—H3	0.9500	C10—H10	0.9500
C4—C5	1.370 (7)	C11—C12	1.379 (7)
C4—H4	0.9500	C11—H11	0.9500
C5—C6	1.383 (7)	C12—C13	1.370 (7)
C5—H5	0.9500	C12—H12	0.9500
C6—H6	0.9500	C13—H13	0.9500
Cl1—O4	1.430 (3)	Cl2—O6	1.425 (4)
Cl1—O3	1.435 (3)	Cl2—O7	1.431 (4)
Cl1—O1	1.442 (3)	Cl2—O8	1.434 (4)
Cl1—O2	1.444 (3)	Cl2—O5	1.439 (4)
C6—N1—C2	120.0 (4)	C13—N3—C9	119.2 (4)
C6—N1—C1	120.2 (4)	C13—N3—C8	119.9 (4)
C2—N1—C1	119.8 (3)	C9—N3—C8	120.9 (3)
N1—C1—H1A	109.5	N3—C8—H8A	109.5
N1—C1—H1B	109.5	N3—C8—H8B	109.5

H1A—C1—H1B	109.5	H8A—C8—H8B	109.5
N1—C1—H1C	109.5	N3—C8—H8C	109.5
H1A—C1—H1C	109.5	H8A—C8—H8C	109.5
H1B—C1—H1C	109.5	H8B—C8—H8C	109.5
N1—C2—C3	121.2 (4)	N3—C9—C10	121.7 (3)
N1—C2—C7	116.7 (4)	N3—C9—C14	117.0 (4)
C3—C2—C7	122.1 (4)	C10—C9—C14	121.3 (4)
C2—C3—C4	118.8 (4)	C9—C10—C11	119.0 (4)
C2—C3—H3	120.6	C9—C10—H10	120.5
C4—C3—H3	120.6	C11—C10—H10	120.5
C5—C4—C3	119.6 (5)	C12—C11—C10	118.7 (5)
C5—C4—H4	120.2	C12—C11—H11	120.7
C3—C4—H4	120.2	C10—C11—H11	120.7
C4—C5—C6	119.6 (4)	C13—C12—C11	120.0 (4)
C4—C5—H5	120.2	C13—C12—H12	120.0
C6—C5—H5	120.2	C11—C12—H12	120.0
N1—C6—C5	120.8 (4)	N3—C13—C12	121.5 (4)
N1—C6—H6	119.6	N3—C13—H13	119.3
C5—C6—H6	119.6	C12—C13—H13	119.3
N2—C7—C2	178.7 (6)	N4—C14—C9	176.8 (5)
O4—Cl1—O3	109.8 (2)	O6—Cl2—O7	110.1 (3)
O4—Cl1—O1	109.3 (2)	O6—Cl2—O8	110.4 (3)
O3—Cl1—O1	109.2 (2)	O7—Cl2—O8	108.3 (2)
O4—Cl1—O2	110.3 (2)	O6—Cl2—O5	109.5 (2)
O3—Cl1—O2	109.3 (2)	O7—Cl2—O5	108.7 (3)
O1—Cl1—O2	109.0 (2)	O8—Cl2—O5	109.8 (2)
C6—N1—C2—C3	0.0 (7)	C13—N3—C9—C10	−0.3 (7)
C1—N1—C2—C3	−178.3 (5)	C8—N3—C9—C10	−177.4 (5)
C6—N1—C2—C7	178.6 (5)	C13—N3—C9—C14	179.9 (4)
C1—N1—C2—C7	0.3 (7)	C8—N3—C9—C14	2.8 (6)
N1—C2—C3—C4	0.1 (8)	N3—C9—C10—C11	0.4 (8)
C7—C2—C3—C4	−178.5 (5)	C14—C9—C10—C11	−179.8 (5)
C2—C3—C4—C5	0.1 (8)	C9—C10—C11—C12	−1.0 (8)
C3—C4—C5—C6	−0.2 (8)	C10—C11—C12—C13	1.5 (8)
C2—N1—C6—C5	−0.1 (7)	C9—N3—C13—C12	0.8 (7)
C1—N1—C6—C5	178.2 (5)	C8—N3—C13—C12	178.0 (5)
C4—C5—C6—N1	0.3 (8)	C11—C12—C13—N3	−1.4 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O1^{i}	0.98	2.53	3.441 (5)	154
C1—H1*C*···O3	0.98	2.52	3.164 (5)	123
C3—H3···O5^{ii}	0.95	2.54	3.326 (5)	140
C5—H5···O8^{iii}	0.95	2.66	3.262 (6)	122
C6—H6···O1^{i}	0.95	2.55	3.415 (6)	152
C6—H6···O4^{i}	0.95	2.65	3.534 (6)	155

C8—H8*A*···O1^{iv}	0.98	2.55	3.294 (6)	132
C8—H8*B*···O7^{v}	0.98	2.57	3.538 (6)	169
C8—H8*C*···O6	0.98	2.51	3.425 (5)	156
C10—H10···O2^{vi}	0.95	2.51	3.367 (5)	150
C12—H12···O2^{vii}	0.95	2.52	3.347 (5)	145
C13—H13···O6	0.95	2.35	3.247 (6)	156

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