1,1′-Methylenebis[4-[(E)-2-(pyridin-4-yl)ethenyl]-pyridinium] dibromide dihydrate

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The chevron-shaped cations of the title hydrated salt, C_{25}H_{22}N_{4^{2+}}/C_{12}Br_{2}/C_{12}H_{2}O, are arranged in back-to-back alternating directions to form a zigzag ribbon propagating along the [010] direction. Intermolecular interactions comprising these ribbons are π–π interactions between the pyridinium and adjacent pyridyl rings, as well as O–H···O hydrogen bonding between water molecules and two adjacent pyridyl N atoms. Half of the cation is generated by the mirror plane. The water O atoms, the central C atom and one Br atom are located on this mirror plane while the other Br atom is on a twofold screw axis.

Structure description

Half of the cation is generated by the mirror plane (x, 1/2 − y, z). The O1, O2, Br1, and Cl atoms are located on this mirror plane and the Br2 atom is on a twofold screw axis (−x, 1/2 + y, −z). The pyridyl–vinyl–pyridinium moiety (Fig. 1) is essentially planar with a 1.7 (3)° dihedral angle between the planes of the pyridinium (N1/C2–C6) and pyridyl (N2/C9–C13) rings. The N1–C1–N1(x, 1/2 − y, z) angle is 110.9 (10)°, which is similar to the N–C–N angles of 111.1 (4) or 112.3 (4)° found in the bromide (Schuster et al. 2022) or PF_{6} (Blanco et al., 2007) salts, respectively, of the 1,1′-methylenebis-4,4′-bipyridinium cation. When two of the title cations are used in a supramolecular cyclic compound with two Pd(ethylenediamine) moieties, the crystal structure had this same N–C–N angle remaining relatively unchanged at 109.1 (19)° and 111.2 (11)° (Blanco et al., 2009).

In the extended structure, the chevron-shaped cations of the title compound arrange in back-to-back alternating directions to form a zigzag ribbon (Fig. 2) propagating along the [010] direction. Water molecules are positioned to interact with the terminal pyridyl nitrogen atom, N2, with an N2–H1D(1/2 − x, 1 − y, 1/2 + z) distance of 2.01 Å (Table 1). The distance between back-to-back pyridinium and pyridyl rings [the closest distance between carbon atoms, C6 of the pyridinium and C13(1 − x, 1 − y, 1 − z) of a pyridyl...
ring, being 3.46 (1) Å (Fig. 2) is suitable for π–π interactions (Sinnokrot et al., 2002), which further consolidate these zigzag ribbons. Water molecules and bromide ions pack between the ribbons (Fig. 3). Other hydrogen-bonded zigzag ribbon structures are observed in 1,3-bis[(tetrahydrofuran-2-yl)methyl]thiourea (Pen˜a et al., 2009) or 1-(4-bromophenyl)-3-(4-ethoxyphenyl)prop-2-en-1-one (Fun et al., 2008).

Synthesis and crystallization

The title compound was synthesized according to published procedures (Blanco et al., 2009). Colorless plates were grown from liquid diffusion of tetrahydrofuran into a dimethylformamide solution of the pyridinium bromide salt.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Disorder of the 4-[((E)-2-(pyridin-4-yl)ethenyl)pyridinium moiety was refined using ‘PART 1’ and ‘PART 2’ with the ratio of occupancies at 47 and 53%. All

Table 1

| Hydrogen-bond geometry (Å, °) | D–H···A | D–H | H···A | D···A | D–H···A |
|-----------------------------|--------|-----|------|------|--------|
| O1–H1C···N2i                  | 0.88   | 2.26| 2.880(11) | 128 |
| O1–H1D···N2ii                 | 0.88   | 2.01| 2.880(11) | 171 |

Symmetry codes: (i) –x + 2, y, –z + 1; (ii) –x + 2, –y + 3, z – 1.

Table 2

| Experimental details. |
|-----------------------|
| Crystal data          |
| Chemical formula      | C_{25}H_{22}N_{4}^{2+}·2Br⁻·2H_{2}O |
| M_r                   | 574.32 |
| Crystal system, space group | Orthorhombic, Pnma |
| Temperature (K)       | 220 |
| a, b, c (Å)           | 15.4863 (2), 22.2936 (3), 7.2100 (1) |
| V (Å³)                | 2489.22 (6) |
| Z                      | 4 |
| Radiation type        | Cu Kα |
| μ (mm⁻¹)              | 4.37 |
| Crystal size (mm)     | 0.04 × 0.03 × 0.02 |
| Data collection       |
| Diffractometer        | XtaLAB Synergy, Dualflex, HyPix |
| Absorption correction | Multi-scan CrysAlis PRO (Rigaku OD, 2021) |
| T_{min}, T_{max}      | 0.671, 1.000 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 25704, 2780, 2439 |
| R_{int}               | 0.030 |
| (sin θ/λ)_{max} (Å⁻¹) | 0.639 |
| Refinement            |
| R[F² > 2σ(F²)], wR(F²), S | 0.036, 0.104, 1.09 |
| No. of reflections    | 2780 |
| No. of parameters     | 244 |
| No. of restraints     | 8 |
| H-atom treatment      | H atoms treated by a mixture of independent and constrained refinement |
| Δρ_{max}, Δρ_{min} (e Å⁻³) | 0.99, −0.86 |

Computer programs: CrysAlis PRO (Rigaku OD, 2021), SHELXT2018/2 (Sheldrick, 2015a), SHELX2018/3 (Sheldrick, 2015b), Mercury (Macrae et al., 2020), and OLEX2 (Dolomanov et al., 2009).
our attempts to refine the structure to achieve equal occupancies led to a drastic worsening of $R_1$ and $wR_2$ values.

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full crystallographic data

1,1′-Methylenebis(4-[(E)-2-(pyridin-4-yl)ethenyl]pyridinium) dibromide dihydrate

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Crystal data

C25H22N4Br2·2H2O  
Mr = 574.32  
Orthorhombic, Pnma  
a = 15.4863 (2) Å  
b = 22.2936 (3) Å  
c = 7.2100 (1) Å  
V = 2489.22 (6) Å³  
Z = 4  
F(000) = 1160

Cu Kα radiation, λ = 1.54184 Å  
θ = 6.1–79.8°  
µ = 4.37 mm⁻¹  
T = 220 K  
Plate, clear light colourless  
0.04 × 0.03 × 0.02 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer  
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source  
Mirror monochromator  
Detector resolution: 10.0000 pixels mm⁻¹  
ω scans  
Absorption correction: multi-scan  
CrysAlisPro (Rigaku OD, 2021)

Refinement

Refinement on F²  
Least-squares matrix: full  
R[F² > 2σ(F²)] = 0.036  
wR(F²) = 0.104  
S = 1.09  
2780 reflections  
244 parameters  
8 restraints

Hydrogen site location: mixed  
H atoms treated by a mixture of independent and constrained refinement

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

|    | x      | y      | z      | U_{iso}/U_{eq} | Occ. (<1) |
|----|--------|--------|--------|----------------|-----------|
| Br1| 0.83013 (2) | 0.250000 | 0.51496 (5) | 0.05780 (16) |
| Br2| 0.500000  | 0.500000 | 0.000000 | 0.06787 (19) |
| O1 | 0.59949 (18) | 0.250000  | −0.0276 (5) | 0.0644 (5) |
| H1C| 0.628097  | 0.228712 | 0.053830 | 0.097* 0.5 |
| H1D| 0.637353  | 0.279127 | −0.030494 | 0.097* 0.5 |
| O2 | 0.61749 (17) | 0.250000  | 0.5693 (5) | 0.0644 (5) |
| H2B| 0.666046  | 0.234075 | 0.534382 | 0.097* 0.5 |
| H2C| 0.616243  | 0.229500 | 0.676421 | 0.097* 0.5 |
| N1 | 0.4441 (7) | 0.3047 (4) | 0.4944 (11) | 0.0280 (19) | 0.471 (7) |
| C2 | 0.4622 (7) | 0.3261 (4) | 0.6635 (9) | 0.0336 (16) | 0.471 (7) |
| H2 | 0.441055  | 0.306491 | 0.769534 | 0.040* 0.471 (7) |
| C3 | 0.5120 (5) | 0.3769 (3) | 0.6814 (7) | 0.0338 (14) | 0.471 (7) |
| H3 | 0.523534  | 0.392117 | 0.800374 | 0.041* 0.471 (7) |
| C4 | 0.5451 (3) | 0.4059 (2) | 0.5289 (9) | 0.0259 (12) | 0.471 (7) |
| C5 | 0.5254 (4) | 0.3821 (3) | 0.3578 (7) | 0.0355 (15) | 0.471 (7) |
| H5 | 0.546674  | 0.400906 | 0.250362 | 0.043* 0.471 (7) |
| C6 | 0.4753 (6) | 0.3316 (4) | 0.3410 (8) | 0.0375 (17) | 0.471 (7) |
| H6 | 0.462840  | 0.315841 | 0.223042 | 0.045* 0.471 (7) |
| N2 | 0.7822 (9) | 0.6508 (4) | 0.5018 (14) | 0.048 (3) | 0.471 (7) |
| C11| 0.7660 (7) | 0.6282 (4) | 0.3350 (11) | 0.0430 (17) | 0.471 (7) |
| H11| 0.788849 | 0.647826 | 0.230565 | 0.052* 0.471 (7) |
| C10| 0.7170 (5) | 0.5769 (3) | 0.3083 (8) | 0.0383 (15) | 0.471 (7) |
| H10| 0.707421  | 0.562561 | 0.187380 | 0.046* 0.471 (7) |
| C9 | 0.6822 (3) | 0.54692 (19) | 0.4566 (10) | 0.0301 (12) | 0.471 (7) |
| C13| 0.6980 (5) | 0.5710 (3) | 0.6290 (8) | 0.0394 (16) | 0.471 (7) |
| H13| 0.674916 | 0.552711 | 0.735506 | 0.047* 0.471 (7) |
| C12| 0.7480 (8) | 0.6224 (4) | 0.6452 (10) | 0.050 (2) | 0.471 (7) |
| H12| 0.758017  | 0.637927 | 0.764548 | 0.060* 0.471 (7) |
| C1 | 0.39067 (17) | 0.250000 | 0.4756 (4) | 0.0281 (5) |
| C7 | 0.5974 (3) | 0.4592 (2) | 0.5575 (7) | 0.0328 (12) | 0.471 (7) |
| H7 | 0.608461 | 0.470689 | 0.680642 | 0.039* 0.471 (7) |
| C8 | 0.6307 (3) | 0.4929 (2) | 0.4239 (6) | 0.0321 (13) | 0.471 (7) |
| H8 | 0.620576  | 0.481388 | 0.300419 | 0.038* 0.471 (7) |
| C8A| 0.6252 (3) | 0.4946 (2) | 0.5660 (6) | 0.0352 (12) | 0.529 (7) |
| H8A| 0.604322  | 0.485675 | 0.685211 | 0.042* 0.529 (7) |
| C7A| 0.6033 (3) | 0.4578 (2) | 0.4290 (6) | 0.0330 (11) | 0.529 (7) |
| H7A| 0.624114  | 0.466670 | 0.309581 | 0.040* 0.529 (7) |
| N1A| 0.4453 (6) | 0.3041 (3) | 0.4673 (9) | 0.0244 (15) | 0.529 (7) |
| C2A| 0.4791 (5) | 0.3212 (3) | 0.3033 (8) | 0.0290 (12) | 0.529 (7) |
| H2A| 0.467537  | 0.298861 | 0.195459 | 0.035* 0.529 (7) |
| C3A| 0.5305 (3) | 0.3713 (2) | 0.2945 (6) | 0.0307 (12) | 0.529 (7) |
| H3A| 0.553479  | 0.383222 | 0.179661 | 0.037* 0.529 (7) |
| C4A| 0.5489 (3) | 0.40443 (19) | 0.4506 (8) | 0.0264 (11) | 0.529 (7) |
| C5A| 0.5131 (4) | 0.3853 (3) | 0.6147 (7) | 0.0341 (13) | 0.529 (7) |
| H5A| 0.523793  | 0.407169 | 0.723830 | 0.041* 0.529 (7) |
C6A  0.4621 (6)  0.3349 (3)  0.6226 (7)  0.0323 (13)  0.529 (7)  
H6A  0.439049  0.322149  0.735640  0.039*  0.529 (7)  
N2A  0.7859 (8)  0.6497 (4)  0.5226 (13)  0.052 (3)  0.529 (7)  
C11A 0.7539 (7)  0.6311 (4)  0.6829 (10)  0.0468 (16)  0.529 (7)  
H11A 0.7011 (4)  0.5811 (3)  0.7003 (7)  0.0401 (14)  0.529 (7)  
N2A  0.7859 (8)  0.6497 (4)  0.5226 (13)  0.052 (3)  0.529 (7)  
C11A 0.7539 (7)  0.6311 (4)  0.6829 (10)  0.0468 (16)  0.529 (7)  
H11A 0.7011 (4)  0.5811 (3)  0.7003 (7)  0.0401 (14)  0.529 (7)  
N2A  0.7859 (8)  0.6497 (4)  0.5226 (13)  0.052 (3)  0.529 (7)  
C11A 0.7539 (7)  0.6311 (4)  0.6829 (10)  0.0468 (16)  0.529 (7)  
H11A 0.7011 (4)  0.5811 (3)  0.7003 (7)  0.0401 (14)  0.529 (7)  

| Br1  | U11  | U22  | U33  | U12  | U13  | U23  |
|------|------|------|------|------|------|------|
| 0.0341 (2) | 0.1080 (4) | 0.03128 (19) | 0.000 | 0.00029 (12) | 0.000 |
| Br2  | 0.1255 (5) | 0.0507 (2) | 0.0274 (2) | 0.0236 (2) | 0.00356 (18) | 0.00004 (13) |
| O1   | 0.0401 (9) | 0.0554 (10) | 0.0978 (16) | 0.000 | −0.0060 (10) | 0.000 |
| O2   | 0.0401 (9) | 0.0554 (10) | 0.0978 (16) | 0.000 | −0.0060 (10) | 0.000 |
| N1   | 0.023 (3) | 0.025 (4) | 0.036 (3) | 0.001 (3) | 0.004 (2) | 0.007 (3) |
| C2   | 0.045 (3) | 0.030 (3) | 0.025 (3) | −0.006 (3) | 0.007 (3) | −0.003 (2) |
| C3   | 0.046 (3) | 0.033 (3) | 0.022 (3) | −0.006 (2) | 0.003 (3) | −0.008 (3) |
| C4   | 0.029 (2) | 0.023 (2) | 0.026 (3) | 0.0000 (16) | 0.002 (2) | −0.004 (3) |
| C5   | 0.048 (3) | 0.033 (3) | 0.025 (4) | −0.002 (2) | 0.008 (3) | 0.008 (3) |
| C6   | 0.051 (4) | 0.036 (3) | 0.026 (3) | −0.003 (3) | −0.010 (3) | −0.004 (3) |
| N2   | 0.039 (6) | 0.025 (6) | 0.078 (6) | 0.000 (5) | 0.003 (5) | 0.007 (5) |
| C1   | 0.042 (3) | 0.028 (3) | 0.060 (4) | −0.005 (2) | 0.005 (3) | 0.006 (3) |
| C10  | 0.040 (3) | 0.035 (3) | 0.040 (4) | −0.002 (2) | 0.004 (3) | −0.001 (3) |
| C9   | 0.028 (2) | 0.023 (2) | 0.039 (4) | 0.0008 (16) | 0.001 (3) | 0.001 (3) |
| C13  | 0.040 (3) | 0.036 (4) | 0.042 (4) | −0.004 (2) | 0.000 (3) | 0.001 (3) |
| C12  | 0.052 (4) | 0.032 (3) | 0.065 (5) | −0.001 (3) | −0.014 (4) | −0.011 (3) |
| C1   | 0.0243 (12) | 0.0240 (11) | 0.0360 (14) | 0.000 | −0.0007 (11) | 0.000 |
| C7   | 0.033 (2) | 0.027 (3) | 0.038 (3) | −0.0030 (19) | 0.0006 (18) | −0.0038 (17) |
| C8   | 0.032 (2) | 0.028 (3) | 0.035 (3) | −0.0021 (19) | −0.0027 (17) | −0.0009 (16) |
| C8A  | 0.0346 (19) | 0.032 (2) | 0.039 (3) | −0.0033 (18) | 0.0025 (16) | 0.0023 (16) |
| C7A  | 0.0326 (19) | 0.029 (2) | 0.037 (2) | −0.0024 (17) | 0.0024 (15) | 0.0007 (16) |
| N1A  | 0.026 (3) | 0.022 (3) | 0.026 (2) | 0.000 (2) | −0.004 (2) | −0.004 (2) |
| C2A  | 0.034 (2) | 0.032 (3) | 0.022 (2) | −0.008 (2) | 0.0000 (18) | 0.0004 (19) |
| C3A  | 0.032 (2) | 0.034 (2) | 0.026 (3) | −0.0048 (18) | 0.004 (2) | 0.003 (2) |
| C4A  | 0.0276 (18) | 0.027 (2) | 0.024 (3) | 0.0010 (14) | −0.001 (2) | −0.008 (2) |
| C5A  | 0.047 (3) | 0.032 (3) | 0.024 (3) | −0.002 (2) | 0.000 (3) | −0.008 (3) |
| C6A  | 0.039 (3) | 0.034 (3) | 0.023 (3) | 0.001 (2) | 0.006 (2) | −0.002 (2) |
| N2A  | 0.041 (5) | 0.033 (6) | 0.081 (5) | −0.010 (5) | −0.001 (5) | −0.007 (5) |
| C11A | 0.045 (3) | 0.035 (3) | 0.061 (4) | −0.006 (2) | −0.007 (3) | −0.007 (3) |
| C10A | 0.042 (2) | 0.034 (3) | 0.044 (3) | −0.001 (2) | −0.006 (3) | 0.000 (3) |
|    | 0.0290 (19) | 0.028 (2) | 0.041 (3) | 0.0021 (16) | −0.001 (2) | −0.003 (3) |
|----|-------------|-----------|-----------|-------------|-----------|-----------|
| C9A| 0.053 (3)   | 0.037 (3) | 0.042 (4) | −0.007 (2)  | 0.005 (3)  | −0.005 (3) |
| C13A| 0.058 (4)  | 0.036 (3) | 0.068 (5) | −0.005 (3)  | 0.017 (4)  | 0.003 (3)  |

**Geometric parameters (Å, °)**

| Bond | Distance (Å) | Angle (°) |
|------|--------------|-----------|
| O1—H1C | 0.8753       |           |
| O1—H1Ci | 0.88 (6)    |           |
| O1—H1D | 0.8752       |           |
| O1—H1Di | 0.88 (8)    |           |
| O1—H1D | 0.8752       |           |
| O1—H1Di | 0.88 (8)    |           |
| O1—H1D | 0.8752       |           |
| O1—H1Di | 0.88 (8)    |           |
| O2—H2B | 0.8688       |           |
| O2—H2B | 0.87 (5)     |           |
| O2—H2C | 0.8975       |           |
| O2—H2C | 0.90 (6)     |           |
| N1—C2 | 1.3385       |           |
| N1—C6 | 1.3481       |           |
| N1—C1 | 1.480 (5)    |           |
| C2—H2 | 0.9400       |           |
| C2—C3 | 1.3755       |           |
| C3—H3 | 0.9400       |           |
| C6—H6 | 0.9400       |           |
| N2—C11 | 1.3275      |           |
| N2—C12 | 1.3235      |           |
| C11—H11 | 0.9400     |           |
| C11—C10 | 1.3868     |           |
| C10—H10 | 0.9400     |           |
| C10—C9 | 1.3715       |           |
| C9—C13 | 1.3756       |           |
| C9—C8 | 1.464 (7)    |           |
| C13—H13 | 0.9400     |           |
| C13—C12 | 1.3883     |           |
| C12—H12 | 0.9400     |           |
| C1—N1A | 1.474 (4)    |           |

| Bond | Angle (°) |
|------|-----------|
| H1C—O1—H1C | 65.7     |
| H1C—O1—H1D | 94.5     |
| H1C—O1—H1D | 94.5     |
| H1D—O1—H1C | 43.5     |
| H1D—O1—H1D | 95.8     |
| H2B—O2—H2B | 48.2     |
| H2B—O2—H2C | 93.4     |
| H2B—O2—H2C | 118.4    |
| Bond/Cross-Bond | 93.4 | C7—C8—C9 | 124.2 (5) |
|----------------|------|-----------|-----------|
| H2B—O2—H2C    | 118.4| C7—C8—H8 | 117.9     |
| H2C—O2—H2Bi   | 61.2 | C7A—C8A—H8A | 117.5 |
| H2C—O2—H2Ci   | 120.9| C7A—C8A—C9A | 125.1 (5) |
| C2—N1—C6      | 119.6 (5) | C9A—C8A—H8A | 117.5 |
| C2—N1—C1      | 119.4 (5) | C8A—C7A—H7A | 117.7 |
| C6—N1—C1      | 120.1 | C8A—C7A—C4A | 124.7 (5) |
| N1—C2—H2      | 119.8 | C4A—C7A—H7A | 117.7 |
| N1—C2—C3      | 120.1 | C2A—N1A—C1 | 119.3 (4) |
| C3—C2—H3      | 119.3 | C6A—N1A—C1 | 119.8 (4) |
| C4—C3—C2      | 121.4 | C6A—N1A—C2A | 120.9 |
| C4—C3—H3      | 119.3 | N1A—C2A—H2A | 120.2 |
| C3—C4—C5      | 117.0 | N1A—C2A—C3A | 119.7 |
| C3—C4—C7      | 118.6 (4) | C3A—C2A—H2A | 120.2 |
| C5—C4—C7      | 124.4 (4) | C2A—C3A—H3A | 119.4 |
| C6—C5—C4      | 121.3 | C2A—C3A—C4A | 121.3 |
| C6—C5—H5      | 119.4 | C4A—C3A—H3A | 119.4 |
| N1—C6—C5      | 119.7 | C3A—C4A—C7A | 117.9 (4) |
| N1—C6—H6      | 120.2 | C5A—C4A—C7A | 125.1 (4) |
| C5—C6—H6      | 120.2 | C5A—C4A—C3A | 117.0 |
| C12—N2—C11    | 116.8 | C6A—C5A—H5A | 119.3 |
| N2—C11—H11    | 118.6 | C6A—C5A—H5A | 119.3 |
| N2—C11—C10    | 122.9 | N1A—C6A—C5A | 119.8 |
| C10—C11—H11   | 118.6 | N1A—C6A—H6A | 120.1 |
| C11—C10—H10   | 119.7 | C5A—C6A—H6A | 120.1 |
| C9—C10—C11    | 120.6 | C11A—N2A—C12A | 116.8 |
| C9—C10—H10    | 119.7 | C11A—N2A—C12A | 116.8 |
| C10—C9—C13    | 116.4 | C12A—N1A—C10A | 123.5 |
| C10—C9—C8     | 119.3 (5) | C10A—C11A—H11A | 118.2 |
| C13—C9—C8     | 124.3 (5) | C11A—C10A—H10A | 120.1 |
| C9—C13—H13    | 120.1 | C9A—C10A—C11A | 119.8 |
| C9—C13—C12    | 119.8 | C9A—C10A—H10A | 120.1 |
| C12—C13—H13   | 120.1 | C10A—C9A—C8A | 119.4 (4) |
| N2—C12—C13    | 123.5 | C13A—C9A—C8A | 124.2 (4) |
| N2—C12—H12    | 118.2 | C13A—C9A—C10A | 116.4 |
| C13—C12—H12   | 118.2 | C9A—C13A—H13A | 119.7 |
| N1—C1—N1      | 110.9 (10) | C9A—C13A—C12A | 120.6 |
| N1—C1—H1A     | 102.9 (11) | C12A—C13A—H13A | 119.7 |
| N1—C1—H1A     | 102.9 (11) | C12A—C13A—H13A | 119.7 |
| N1—C1—H1B     | 110.9 (11) | N2A—C12A—C13A | 122.8 |
| N1—C1—H1B     | 110.9 (11) | N2A—C12A—H12A | 118.6 |
| N1A—C1—N1A    | 109.8 (9) | C13A—C12A—H12A | 118.6 |
| N1—C2—C3—C4   | -1.2 | C7—C4—C5—C6 | -179.8 (6) |
| C2—N1—C6—C5   | -0.9 | C8—C9—C13—C12 | 179.8 (6) |
| C2—N1—C1—N1'  | -84.1 (7) | C8A—C7A—C4A—C3A | 178.8 (4) |
| C2—C3—C4—C5   | 0.7 | C8A—C7A—C4A—C5A | 0.2 (6) |
C2—C3—C4—C7  −179.8 (6)  C8A—C9A—C13A—C12A  −178.8 (6)
C3—C4—C5—C6  −0.3  C7A—C8A—C9A—C10A  −176.9 (4)
C3—C4—C7—C8  −177.3 (5)  C7A—C8A—C9A—C13A  2.7 (7)
C4—C5—C6—N1  0.4  C7A—C4A—C5A—C6A  179.4 (5)
C4—C7—C8—C9  179.1 (4)  N1A—C1—N1A—C2A  76.4 (7)
C3—C4—C7—C8  0.3  C7A—C8A—C9A—C13A  −102.3 (5)
C6—N1—C1—N1i  94.7 (7)  C2A—N1A—C6A—C5A  1.2
N2—C11—C10—C9  0.2  C2A—C3A—C4A—C7A  −179.2 (5)
C11—N2—C12—C13  0.7  C2A—C3A—C4A—C5A  −0.5
C11—C10—C9—C8  0.8  C3A—C4A—C5A—C6A  0.8
C11—C10—C9—C8  180.0 (6)  C4A—C5A—C6A—N1A  −1.2
C10—C9—C13—C12  −1.1  C6A—N1A—C2A—C3A  −0.9
C10—C9—C8—C7  177.0 (5)  N2A—C11A—C10A—C9A  0.0
C9—C13—C12—N2  0.3  C11A—N2A—C12A—C13A  −1.1
C13—C9—C8—C7  −3.9 (7)  C11A—C10A—C9A—C8A  178.7 (6)
C12—N2—C11—C10  −1.0  C11A—C10A—C9A—C13A  −1.0
C1—N1—C2—C3  180.0 (10)  C10A—C9A—C13A—C12A  0.8
C1—N1—C6—C5  −179.6 (9)  C9A—C8A—C7A—C4A  −180.0 (4)
C1—N1A—C2A—C3A  −179.6 (8)  C9A—C13A—C12A—N2A  0.2
C1—N1A—C6A—C5A  179.9 (8)  C12A—N2A—C11A—C10A  1.0

Symmetry code: (i) x, −y+1/2, z.

Hydrogen-bond geometry (Å, °)

| D—H···A  | D—H | H···A | D···A  | D—H···A |
|---------|------|-------|--------|---------|
| O1—H1C—N2ii | 0.88 | 2.26  | 2.880 (11) | 128   |
| O1—H1D—N2iii | 0.88 | 2.01  | 2.880 (11) | 171   |

Symmetry codes: (ii) −x+3/2, y−1/2, z−1/2; (iii) −x+3/2, −y+1, z−1/2.