

Crystal structure of 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-a]quinoxalin-11-ium dibromide

Md. Serajul Haque Faizi,^a Natalia O. Sharkina^{b*} and Turganbay S. Iskenderov^b

^aDepartment of Chemistry, Indian Institute of Technology Kanpur, Kanpur, UP 208 016, India, and ^bNational Taras Shevchenko University, Department of Chemistry, Volodymyrska str. 64, 01601 Kyiv, Ukraine. *Correspondence e-mail: nsharkina@ukr.net

Received 2 November 2014; accepted 27 November 2014

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

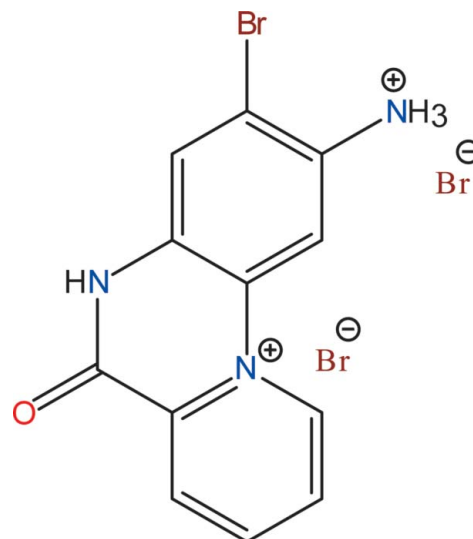
The title salt, $C_{12}H_{10}BrN_3O^{2+} \cdot 2Br^-$, was synthesized from the reaction of N^1, N^4 -bis(pyridin-2-ylmethylidene)benzene-1,4-diamine and bromine in a methanol solution. All non-H atoms of the 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-*a*]quinoxalin-11-ium cation are nearly coplanar, the maximum deviation being 0.114 (4) Å. In the crystal, the cations and anions are linked through N—H...Br hydrogen bonds and weak C—H...Br interactions, forming a three-dimensional supramolecular architecture. A short Br...Br contact [3.3088 (9) Å] is observed in the crystal.

Keywords: crystal structure; bromide; pyrido[1,2-*a*]quinoxalin-11-ium; C—H...Br interactions.

CCDC reference: 1036569

1. Related literature

For applications of quinoxalines, see: Duffy *et al.* (2002); Gazit *et al.* (1996); Harmenberg *et al.* (1991); Naylor *et al.* (1993). For types of quinoxalines and a structure similar to title compound, see: Eiden & Peter (1966); Koner & Ray (2008); Fritsky *et al.* (2006); Kanderl *et al.* (2005); Moroz *et al.* (2012). For background to and applications of related compounds, see: Faizi & Sen (2014); Faizi *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_{12}H_{10}BrN_3O^{2+} \cdot 2Br^-$
 $M_r = 451.96$
 Monoclinic, $P2_1/c$
 $a = 5.6782$ (2) Å
 $b = 11.9822$ (4) Å
 $c = 20.2528$ (7) Å
 $\beta = 90.891$ (2)°

$V = 1377.78$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 8.78$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.25 \times 0.20$ mm

2.2. Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{min} = 0.178$, $T_{max} = 0.273$

14369 measured reflections
 2424 independent reflections
 1804 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.106$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.130$
 $S = 0.97$
 2424 reflections

173 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.23$ e Å⁻³
 $\Delta\rho_{min} = -0.88$ e Å⁻³

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...Br1 ⁱ	0.88	2.46	3.322 (5)	167
N3—H1N3...Br2 ⁱⁱ	0.91	2.53	3.432 (5)	171
N3—H2N3...Br2 ⁱⁱⁱ	0.91	2.42	3.287 (5)	160
N3—H3N3...Br1	0.91	2.50	3.374 (5)	162
C2—H2...Br2 ^{iv}	0.95	2.91	3.813 (6)	160
C3—H3...Br1 ^v	0.95	2.85	3.752 (7)	160
C8—H8...Br1 ⁱ	0.95	2.86	3.672 (6)	144
C11—H11...Br2 ⁱⁱ	0.95	2.80	3.639 (6)	148

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $x + 1, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (v) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve

structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenberg & Putz, 2006); software used to prepare material for publication: *DIAMOND*.

Acknowledgements

The authors are grateful to the Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, UP 208 016, India, for X-ray data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5829).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Brandenberg, K. & Putz, H. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2003). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Duffy, K. J., Haltiwanger, R. C., Freyer, A. J., Li, F., Luengo, J. I. & Cheng, H.-Y. (2002). *J. Chem. Soc. Perkin Trans. 2*, pp. 181–185.
- Eiden, F. & Peter, P. (1966). *Arch. Pharm. Pharm. Med. Chem.* **299**, 139–146.
- Faizi, M. S. H., Mashrai, A., Shahid, M. & Ahmad, M. (2014). *Acta Cryst.* **E70**, o806.
- Faizi, M. S. H. & Sen, P. (2014). *Acta Cryst.* **E70**, m206–m207.
- Fritsky, I. O., Kozłowski, H., Kandal, O. M., Haukka, M., Świątek-Kozłowska, J., Gumienna-Kontecka, E. & Meyer, F. (2006). *Chem. Commun.* pp. 4125–4127.
- Gazit, A., App, H., McMahon, G., Chen, J., Levitzki, A. & Bohmer, F. D. (1996). *J. Med. Chem.* **39**, 2170–2177.
- Harmenberg, J., Åkesson-Johansson, A., Gråslund, A., Malmfors, T., Bergman, J., Wahren, B., Åkerfeldt, S., Lundblad, L. & Cox, S. (1991). *Antiviral Res.* **15**, 193–204.
- Kandal, O. M., Kozłowski, H., Dobosz, A., Swiatek-Kozłowska, J., Meyer, F. & Fritsky, I. O. (2005). *Dalton Trans.* pp. 1428–1437.
- Koner, R. R. & Ray, M. (2008). *Inorg. Chem.* **47**, 9122–9124.
- Moroz, Y. S., Demeshko, S., Haukka, M., Mokhir, A., Mitra, U., Stocker, M., Müller, P., Meyer, F. & Fritsky, I. O. (2012). *Inorg. Chem.* **51**, 7445–7447.
- Naylor, M. A., Stephens, M. A., Nolan, J., Sutton, B., Tocher, J. H., Fielden, E. M., Adams, G. E. & Stratford, I. J. (1993). *Anticancer Drug. Des.* **8**, 439–461.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2015). E71, o17–o18 [doi:10.1107/S2056989014026127]

Crystal structure of 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-*a*]quinoxalin-11-ium dibromide

Md. Serajul Haque Faizi, Natalia O. Sharkina and Turganbay S. Iskenderov

S1. Comment

Quinoxalines are an important class of heterocyclic compounds, some of which are found to be useful as fluorophores, dyes, and antibiotics (Duffy *et al.*, 2002; Gazit *et al.*, 1996). Many drug candidates bearing quinoxaline core structures are in clinical trials in antiviral, anticancer and CNS (central nervous system) therapeutic areas (Harmenberg *et al.*, 1991; Naylor *et al.*, 1993). The present work is a part of an ongoing structural study of Schiff bases and their utilization in the synthesis of previously unknown organic and polynuclear coordination compounds (Faizi & Sen, 2014; Faizi *et al.*, 2014; Moroz *et al.*, 2012), and we report here synthesis and structure of 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-*a*]quinoxalin-11-ium bromide (ABODQ). There are very few examples similar to title compound have been reported in the literature (Eiden & Peter, 1966).

The title compound was synthesized from the reaction of two equimolar amounts of molecular bromine and pyridine derivative Schiff base *N1,N4*-bis(pyridine-2-ylmethylene) benzene-1,4-diamine (BPYBD). The cyclization occurs by oxidation of BPYBD, reduction of molecular bromine and finally hydrolysis of the imine bond which creates the dication at two of the nitrogen atoms in the quinoxaline ring system.

In the structure of the title bromide salt, the dication is essentially planar with a longer C10—N3 distance of 1.45 (3) Å, compared to the usual C_{aro}—N_{amine} single bond distance of 1.43 (3) Å. This might be due to the electron withdrawing effect of positively charged pyridine, which increased the C—N_{amine} bond order. Other C—C and C—N bond distances are well within the limits expected for aromatic rings (Koner & Ray, 2008; Kanderl *et al.*, 2005; Fritsky *et al.*, 2006).

The asymmetric unit contains a discrete 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-*a*]quinoxalin-11-ium cation, with a protonated amine, pyridine group, and two bromide anion (Fig 1). In title compound, the ions are connected into a three dimensional hydrogen-bonded network *via* N—H \cdots Br and C—H \cdots Br hydrogen bonds (Table 1). All H_{ammonium} atoms and H_{pyrazine} N—H group are involved in hydrogen bonds with two different bromide ions, and each anion accepts hydrogen bonds from three different cations. No intermolecular π – π interactions are evident in the hydrocarbon layer in title compound.

S2. Experimental

Molecular bromine (220 mg, 72.0 mL, 1.40 mmol) was added to a methanolic solution (10 ml) of Schiff base, *N1,N4*-bis(pyridine-2-ylmethylene)benzene-1,4-diamine (BPYBD) (197 mg, 0.70 mmol). The color of the solution was immediately changed from yellow to orange. The reaction mixture was stirred for 4 h at room temperature under hood. The resulting yellow precipitate was recovered by filtration, washed several times with a small portions of acetone and then with diethyl ether to give 200 mg (64%) of 2-azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido [1,2-*a*]quinoxalin-11-ium bromide (ABODQ). The crystal of the title compound suitable for X-ray analysis was obtained within 3 days by slow evaporation of the methanol solvent.

S3. Refinement

H atoms were placed in calculated positions and treated as riding on their parent atoms with C—H = 0.95 Å, N—H = 0.88 or 0.91 Å. $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$ for the amino-H atoms and $1.2U_{\text{eq}}(\text{C}, \text{N})$ for the others.

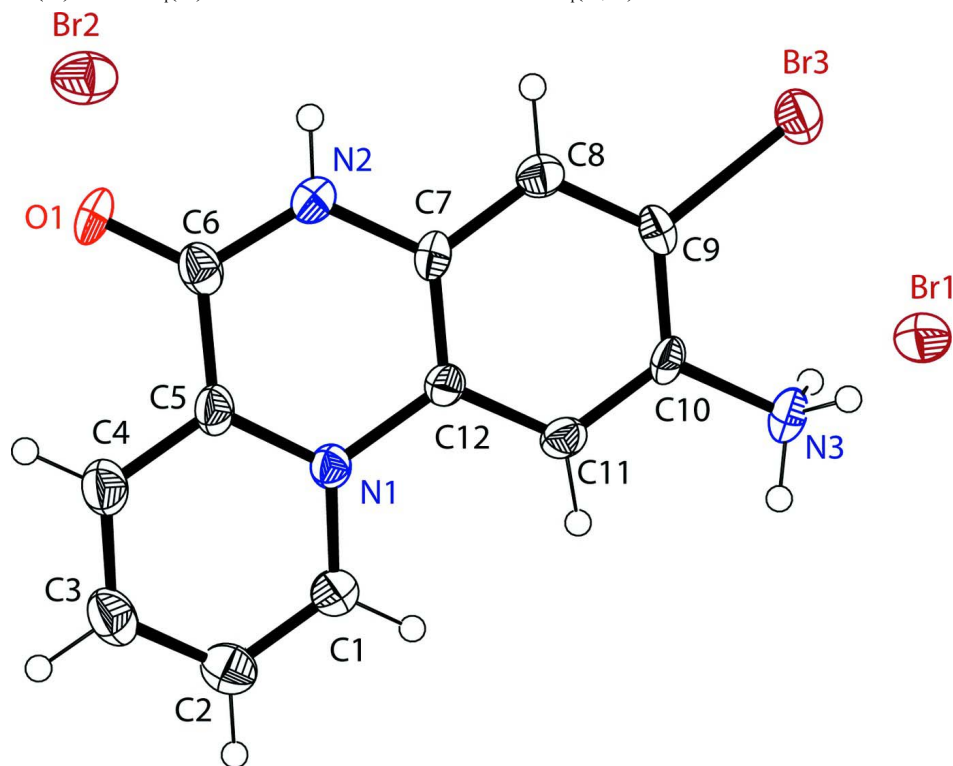


Figure 1

The molecular conformation and atom-numbering scheme for the title compound, with non-H atoms drawn as 40% probability displacement ellipsoids.

2-Azaniumyl-3-bromo-6-oxo-5,6-dihydropyrido[1,2-a]quinoxalin-11-ium dibromide

Crystal data

$\text{C}_{12}\text{H}_{10}\text{BrN}_3\text{O}^{2+} \cdot 2\text{Br}^-$

$M_r = 451.96$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.6782(2) \text{ \AA}$

$b = 11.9822(4) \text{ \AA}$

$c = 20.2528(7) \text{ \AA}$

$\beta = 90.891(2)^\circ$

$V = 1377.78(8) \text{ \AA}^3$

$Z = 4$

$F(000) = 864$

$D_x = 2.179 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 999 reflections

$\theta = 2.6\text{--}28.6^\circ$

$\mu = 8.78 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, yellow

$0.30 \times 0.25 \times 0.20 \text{ mm}$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\text{min}} = 0.178$, $T_{\text{max}} = 0.273$

14369 measured reflections

2424 independent reflections

1804 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.106$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -6 \rightarrow 6$

$k = -14 \rightarrow 14$
 $l = -23 \rightarrow 24$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.130$
 $S = 0.97$
 2424 reflections
 173 parameters
 0 restraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0801P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.88 \text{ e } \text{\AA}^{-3}$

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. 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.1684 (11)	0.3466 (5)	0.6250 (3)	0.0348 (16)
H1	1.1805	0.3779	0.5821	0.042*
C2	1.3279 (12)	0.3771 (5)	0.6724 (3)	0.0404 (17)
H2	1.4479	0.4297	0.6628	0.049*
C3	1.3135 (12)	0.3313 (6)	0.7341 (3)	0.0432 (18)
H3	1.4246	0.3511	0.7676	0.052*
C4	1.1375 (12)	0.2564 (6)	0.7472 (3)	0.0408 (17)
H4	1.1293	0.2230	0.7896	0.049*
C5	0.9719 (11)	0.2291 (5)	0.6989 (3)	0.0308 (15)
C6	0.7750 (11)	0.1557 (5)	0.7166 (3)	0.0327 (15)
C7	0.6487 (11)	0.1672 (5)	0.6019 (3)	0.0284 (14)
C8	0.4824 (11)	0.1344 (5)	0.5543 (3)	0.0297 (14)
H8	0.3582	0.0851	0.5655	0.036*
C9	0.5012 (11)	0.1750 (5)	0.4905 (3)	0.0287 (14)
C10	0.6803 (11)	0.2482 (5)	0.4745 (3)	0.0272 (14)
C11	0.8407 (11)	0.2812 (5)	0.5212 (3)	0.0294 (14)
H11	0.9619	0.3323	0.5104	0.035*
C12	0.8249 (11)	0.2387 (5)	0.5857 (3)	0.0252 (14)
N1	0.9939 (8)	0.2736 (4)	0.6368 (2)	0.0262 (11)
N2	0.6287 (9)	0.1254 (4)	0.6658 (2)	0.0319 (12)
H2A	0.5160	0.0770	0.6737	0.038*
N3	0.6987 (9)	0.2912 (4)	0.4080 (2)	0.0343 (13)

H1N3	0.8278	0.3360	0.4054	0.052*
H2N3	0.5673	0.3314	0.3976	0.052*
H3N3	0.7126	0.2334	0.3792	0.052*
O1	0.7430 (8)	0.1251 (4)	0.7735 (2)	0.0428 (12)
Br1	0.82448 (12)	0.04974 (5)	0.33038 (3)	0.0399 (2)
Br2	0.21399 (13)	0.05913 (6)	0.91141 (4)	0.0478 (3)
Br3	0.26693 (12)	0.12868 (6)	0.42784 (3)	0.0388 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (4)	0.036 (4)	0.033 (4)	−0.004 (3)	0.000 (3)	0.003 (3)
C2	0.038 (4)	0.036 (4)	0.047 (4)	−0.002 (3)	−0.002 (3)	−0.002 (3)
C3	0.038 (5)	0.053 (5)	0.038 (4)	0.003 (4)	−0.005 (3)	−0.015 (4)
C4	0.039 (4)	0.053 (4)	0.030 (4)	0.001 (3)	−0.002 (3)	−0.007 (3)
C5	0.031 (4)	0.040 (4)	0.021 (3)	0.004 (3)	0.002 (3)	−0.005 (3)
C6	0.030 (4)	0.040 (4)	0.028 (4)	0.006 (3)	−0.002 (3)	−0.008 (3)
C7	0.036 (4)	0.031 (4)	0.018 (3)	0.002 (3)	0.002 (3)	−0.001 (3)
C8	0.026 (4)	0.031 (3)	0.032 (4)	0.001 (3)	0.004 (3)	0.000 (3)
C9	0.029 (4)	0.033 (3)	0.024 (3)	0.004 (3)	−0.008 (3)	−0.005 (3)
C10	0.030 (4)	0.035 (4)	0.016 (3)	0.005 (3)	0.006 (2)	−0.002 (3)
C11	0.023 (4)	0.035 (4)	0.030 (3)	−0.002 (3)	0.007 (3)	−0.002 (3)
C12	0.026 (4)	0.027 (3)	0.022 (3)	0.000 (3)	0.003 (3)	−0.002 (3)
N1	0.026 (3)	0.030 (3)	0.023 (3)	0.001 (2)	0.001 (2)	−0.002 (2)
N2	0.033 (3)	0.037 (3)	0.026 (3)	−0.002 (2)	0.005 (2)	0.002 (2)
N3	0.041 (4)	0.043 (3)	0.020 (3)	0.005 (2)	0.004 (2)	0.002 (2)
O1	0.050 (3)	0.062 (3)	0.016 (2)	−0.007 (2)	0.008 (2)	0.004 (2)
Br1	0.0317 (5)	0.0464 (5)	0.0415 (4)	−0.0044 (3)	0.0032 (3)	−0.0017 (3)
Br2	0.0423 (5)	0.0435 (5)	0.0579 (5)	−0.0028 (3)	0.0115 (4)	−0.0072 (3)
Br3	0.0370 (5)	0.0460 (5)	0.0333 (4)	0.0011 (3)	−0.0044 (3)	−0.0048 (3)

Geometric parameters (Å, °)

C1—N1	1.346 (7)	C7—N2	1.394 (7)
C1—C2	1.359 (9)	C8—C9	1.387 (8)
C1—H1	0.9500	C8—H8	0.9500
C2—C3	1.368 (9)	C9—C10	1.385 (9)
C2—H2	0.9500	C9—Br3	1.907 (6)
C3—C4	1.372 (10)	C10—C11	1.362 (8)
C3—H3	0.9500	C10—N3	1.449 (7)
C4—C5	1.384 (8)	C11—C12	1.405 (8)
C4—H4	0.9500	C11—H11	0.9500
C5—N1	1.374 (7)	C12—N1	1.462 (7)
C5—C6	1.471 (9)	N2—H2A	0.8800
C6—O1	1.225 (7)	N3—H1N3	0.9100
C6—N2	1.361 (8)	N3—H2N3	0.9100
C7—C12	1.361 (8)	N3—H3N3	0.9100
C7—C8	1.395 (8)		

N1—C1—C2	122.3 (6)	C8—C9—C10	120.5 (6)
N1—C1—H1	118.9	C8—C9—Br3	117.1 (5)
C2—C1—H1	118.9	C10—C9—Br3	122.4 (4)
C1—C2—C3	119.2 (7)	C11—C10—C9	120.5 (5)
C1—C2—H2	120.4	C11—C10—N3	119.0 (6)
C3—C2—H2	120.4	C9—C10—N3	120.5 (5)
C2—C3—C4	119.6 (6)	C10—C11—C12	119.2 (6)
C2—C3—H3	120.2	C10—C11—H11	120.4
C4—C3—H3	120.2	C12—C11—H11	120.4
C3—C4—C5	120.4 (6)	C7—C12—C11	120.7 (6)
C3—C4—H4	119.8	C7—C12—N1	119.1 (5)
C5—C4—H4	119.8	C11—C12—N1	120.2 (5)
N1—C5—C4	119.0 (6)	C1—N1—C5	119.5 (5)
N1—C5—C6	122.3 (5)	C1—N1—C12	122.5 (5)
C4—C5—C6	118.7 (6)	C5—N1—C12	118.0 (5)
O1—C6—N2	122.2 (6)	C6—N2—C7	123.2 (5)
O1—C6—C5	122.1 (6)	C6—N2—H2A	118.4
N2—C6—C5	115.7 (5)	C7—N2—H2A	118.4
C12—C7—C8	120.2 (5)	C10—N3—H1N3	109.5
C12—C7—N2	121.4 (5)	C10—N3—H2N3	109.5
C8—C7—N2	118.5 (6)	H1N3—N3—H2N3	109.5
C9—C8—C7	119.0 (6)	C10—N3—H3N3	109.5
C9—C8—H8	120.5	H1N3—N3—H3N3	109.5
C7—C8—H8	120.5	H2N3—N3—H3N3	109.5
N1—C1—C2—C3	0.9 (10)	N2—C7—C12—C11	-179.2 (5)
C1—C2—C3—C4	-0.7 (11)	C8—C7—C12—N1	178.6 (5)
C2—C3—C4—C5	-1.5 (11)	N2—C7—C12—N1	-1.1 (9)
C3—C4—C5—N1	3.4 (10)	C10—C11—C12—C7	-1.4 (9)
C3—C4—C5—C6	-175.0 (6)	C10—C11—C12—N1	-179.5 (5)
N1—C5—C6—O1	-172.7 (6)	C2—C1—N1—C5	1.1 (9)
C4—C5—C6—O1	5.7 (9)	C2—C1—N1—C12	-178.7 (6)
N1—C5—C6—N2	6.4 (8)	C4—C5—N1—C1	-3.2 (9)
C4—C5—C6—N2	-175.2 (6)	C6—C5—N1—C1	175.2 (5)
C12—C7—C8—C9	0.6 (9)	C4—C5—N1—C12	176.5 (5)
N2—C7—C8—C9	-179.7 (5)	C6—C5—N1—C12	-5.1 (8)
C7—C8—C9—C10	-0.9 (9)	C7—C12—N1—C1	-178.0 (6)
C7—C8—C9—Br3	-179.4 (4)	C11—C12—N1—C1	0.1 (9)
C8—C9—C10—C11	0.1 (9)	C7—C12—N1—C5	2.3 (8)
Br3—C9—C10—C11	178.4 (4)	C11—C12—N1—C5	-179.6 (5)
C8—C9—C10—N3	-179.5 (5)	O1—C6—N2—C7	174.0 (6)
Br3—C9—C10—N3	-1.1 (8)	C5—C6—N2—C7	-5.1 (8)
C9—C10—C11—C12	1.1 (9)	C12—C7—N2—C6	2.7 (9)
N3—C10—C11—C12	-179.3 (5)	C8—C7—N2—C6	-177.0 (5)
C8—C7—C12—C11	0.6 (9)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 <i>A</i> \cdots Br1 ⁱ	0.88	2.46	3.322 (5)	167
N3—H1 <i>N</i> 3 \cdots Br2 ⁱⁱ	0.91	2.53	3.432 (5)	171
N3—H2 <i>N</i> 3 \cdots Br2 ⁱⁱⁱ	0.91	2.42	3.287 (5)	160
N3—H3 <i>N</i> 3 \cdots Br1	0.91	2.50	3.374 (5)	162
C2—H2 \cdots Br2 ^{iv}	0.95	2.91	3.813 (6)	160
C3—H3 \cdots Br1 ^v	0.95	2.85	3.752 (7)	160
C8—H8 \cdots Br1 ⁱ	0.95	2.86	3.672 (6)	144
C11—H11 \cdots Br2 ⁱⁱ	0.95	2.80	3.639 (6)	148

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, -y+1/2, z-1/2$; (iii) $x, -y+1/2, z-1/2$; (iv) $-x+2, y+1/2, -z+3/2$; (v) $x+1, -y+1/2, z+1/2$.