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1-Benzyl-3-methylimidazolium bromide

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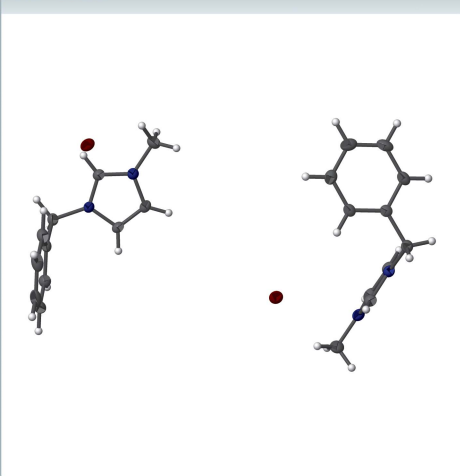
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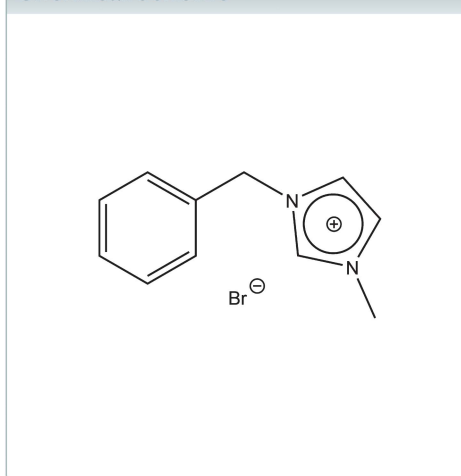
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, (BenzMIm)Br (BenzMIm=1-benzyl-3-methylimidazolium), $C_{11}H_{13}N_2^+ \cdot Br^-$, was obtained as single crystals directly from a pure and liquid sample of the compound over several weeks. The molecular structure of (BenzMIm)Br consists of separated bromide anions and 1-benzyl-3-methylimidazolium cations connected *via* short C—H...Br contacts. The compound exhibits a relatively low melting point (m.p. = 72°C) and is a supercooled, highly viscous transparent liquid at ambient conditions. The title compound crystallizes with two unique ion pairs in the asymmetric unit of the orthorhombic unit cell.

3D view



Chemical scheme



Structure description

For the last 20 years, ionic liquids as salts with low melting points have attracted great interest because of their unique properties and applications. These properties include, for instance, large liquid ranges, broad electrochemical windows as well as low vapor pressures (Hallett & Welton, 2011; Welton, 1999). The title compound, which is a useful starting material in our ongoing efforts to investigate metal-containing ionic liquids (Peppel *et al.*, 2010; Peppel *et al.*, 2017; Peppel *et al.*, 2019) was obtained as single crystals over a period of several weeks directly from its pure, highly viscous and supercooled liquid. 1-Benzyl-3-methylimidazolium bromide expands the range of known single-crystal X-ray structures of ionic liquids of the general formula (BenzMIm)*X* (*X* = Cl, PF₆ (Ji *et al.*, 2010; Hillesheim & Scipione, 2014) with a third example (*X* = Br). It can be seen from Fig. 1 that the (BenzMIm)Br is characterized by discrete 1-benzyl-3-methylimidazolium cations and bromide anions. The shortest C—H...Br contacts equal 2.740 Å (sum of van der Waals radii for H and Br: 3.0 Å). All bond lengths and angles within the cation are in expected ranges (Leclercq *et al.*, 2009). The two symmetry-independent molecular units mainly differ by the angle between the phenyl and the imidazolium ring which is 84.02 (7)° in one of the cations and to 80.47 (7)° in the other. The title compound



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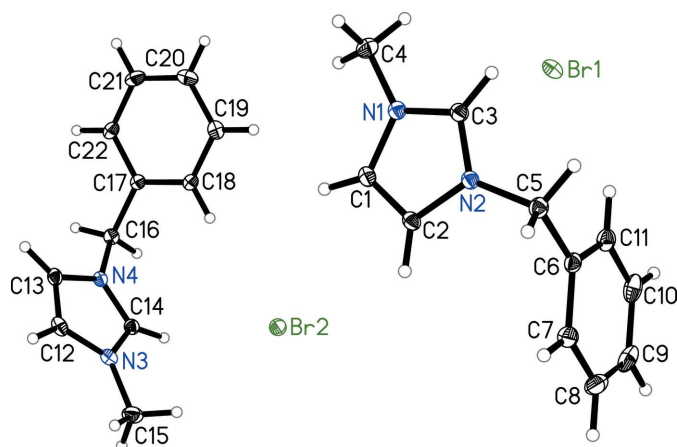


Figure 1
Molecular structure of the title compound. Displacement ellipsoids correspond to 30% probability.

crystallizes with two unique ion pairs in the asymmetric unit of the orthorhombic unit cell.

Synthesis and crystallization

The title compound, (BenzMIm)Br, was obtained in high purity as a transparent, supercooled, highly viscous liquid in multi-gram scale from *N*-methylimidazole and benzyl bromide in ethyl acetate solution under ambient conditions. Benzyl bromide (15.0 g, 87.7 mmol) was added in one portion to a vigorously stirred solution of *N*-methylimidazole (5.0 g, 60.9 mmol) in 100 ml ethyl acetate at room temperature. The clear solution became turbid after a few minutes and was stirred at room temperature overnight. Afterwards, the product was washed several times with portions of ethyl acetate and dried *in vacuo* ($T = 90^\circ\text{C}$, $p = 20$ mbar, yield: 13.1 g, 85%).

Analytic data for (BenzMIm)Br: m.p. 72°C , EA for $\text{C}_{11}\text{H}_{13}\text{BrN}_2$ % (calc.): C 52.47 (52.19); H 4.93 (5.18); N 10.91 (11.07); Br 31.63 (31.56).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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Table 1

Experimental details.

Crystal data	
Chemical formula	$\text{C}_{11}\text{H}_{13}\text{N}_2^+\cdot\text{Br}^-$
M_r	253.14
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	150
a, b, c (Å)	10.9070 (8), 18.8993 (14), 21.6608 (15)
V (Å ³)	4465.0 (6)
Z	16
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.65
Crystal size (mm)	0.40 × 0.32 × 0.22
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
$T_{\min}$, $T_{\max}$	0.33, 0.51
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	51842, 5934, 5054
R_{int}	0.028
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.682
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.051, 1.03
No. of reflections	5934
No. of parameters	255
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.32, -0.32

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *XP* in *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

References

- Bruker (2013). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2014). *APEX2* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Hallett, J. P. & Welton, T. (2011). *Chem. Rev.* **111**, 3508–3576.
- Hillesheim, P. C. & Scipione, K. A. (2014). *Acta Cryst.* **E70**, o1248–o1249.
- Ji, X., Cheng, B., Song, J. & Liu, C. (2010). *Acta Cryst.* **E66**, o218.
- Leclercq, L., Simard, M. & Schmitzer, A. R. (2009). *J. Mol. Struct.* **918**, 101–107.
- Peppel, T., Geppert-Rybczyńska, M., Neise, C., Kragl, U. & Köckerling, M. (2019). *Materials* **12**, 3764.
- Peppel, T., Hinz, A., Thiele, P., Geppert-Rybczyńska, M., Lehmann, J. K. & Köckerling, M. (2017). *Eur. J. Inorg. Chem.* pp. 885–893.
- Peppel, T., Köckerling, M., Geppert-Rybczyńska, M., Ralys, R. V., Lehmann, J. K., Verevkin, S. P. & Heintz, A. (2010). *Angew. Chem. Int. Ed.* **49**, 7116–7119.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Welton, T. (1999). *Chem. Rev.* **99**, 2071–2084.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2020). **5**, x200768 [https://doi.org/10.1107/S2414314620007683]

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Crystal data

$C_{11}H_{13}N_2^+ \cdot Br^-$

$M_r = 253.14$

Orthorhombic, *Pbca*

$a = 10.9070$ (8) Å

$b = 18.8993$ (14) Å

$c = 21.6608$ (15) Å

$V = 4465.0$ (6) Å³

$Z = 16$

$F(000) = 2048$

$D_x = 1.506$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9498 reflections

$\theta = 2.4\text{--}30.4^\circ$

$\mu = 3.65$ mm⁻¹

$T = 150$ K

Prism, colourless

$0.40 \times 0.32 \times 0.22$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 8.3333 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

$T_{\min} = 0.33$, $T_{\max} = 0.51$

51842 measured reflections

5934 independent reflections

5054 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 29.0^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -14 \rightarrow 14$

$k = -25 \rightarrow 25$

$l = -29 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.051$

$S = 1.03$

5934 reflections

255 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2 + 1.6832P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.31$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.22716 (2)	0.01486 (2)	0.46713 (2)	0.02635 (4)
Br2	0.78396 (2)	0.20634 (2)	0.71589 (2)	0.02478 (4)
C1	0.17556 (12)	0.07637 (7)	0.67512 (6)	0.0210 (3)
H1	0.234951	0.076170	0.707203	0.025*
C2	0.10465 (12)	0.13162 (7)	0.65814 (6)	0.0205 (3)
H2	0.104466	0.177529	0.676007	0.025*
C3	0.05902 (12)	0.04116 (7)	0.59817 (6)	0.0204 (3)
H3	0.022230	0.012662	0.567154	0.024*
C4	0.19785 (14)	−0.05091 (8)	0.63992 (7)	0.0286 (3)
H4A	0.147699	−0.080564	0.667121	0.043*
H4B	0.281713	−0.048522	0.656022	0.043*
H4C	0.198986	−0.071406	0.598363	0.043*
C5	−0.05432 (12)	0.15224 (7)	0.57392 (6)	0.0228 (3)
H5A	−0.118776	0.170949	0.601653	0.027*
H5B	−0.094422	0.122786	0.541970	0.027*
C6	0.01252 (12)	0.21301 (7)	0.54350 (6)	0.0213 (3)
C7	0.00238 (14)	0.28059 (8)	0.56795 (7)	0.0271 (3)
H7	−0.048238	0.288620	0.602946	0.033*
C8	0.06598 (14)	0.33662 (8)	0.54144 (8)	0.0337 (3)
H8	0.058858	0.382779	0.558435	0.040*
C9	0.13959 (14)	0.32536 (9)	0.49039 (8)	0.0349 (4)
H9	0.183155	0.363715	0.472431	0.042*
C10	0.14976 (13)	0.25800 (9)	0.46543 (7)	0.0332 (3)
H10	0.199832	0.250330	0.430171	0.040*
C11	0.08660 (13)	0.20158 (8)	0.49200 (6)	0.0261 (3)
H11	0.094021	0.155416	0.475052	0.031*
C12	0.86546 (12)	0.13770 (8)	0.92679 (6)	0.0247 (3)
H12	0.807687	0.143230	0.959254	0.030*
C13	0.93090 (12)	0.07900 (8)	0.91414 (6)	0.0231 (3)
H13	0.928098	0.035409	0.935940	0.028*
C14	0.98114 (12)	0.16068 (7)	0.84610 (6)	0.0216 (3)
H14	1.018734	0.184442	0.812405	0.026*
C15	0.84898 (15)	0.26012 (8)	0.87971 (7)	0.0327 (3)
H15A	0.910658	0.293794	0.894524	0.049*
H15B	0.774922	0.264014	0.905102	0.049*
H15C	0.828730	0.270763	0.836621	0.049*
C16	1.08871 (12)	0.04543 (7)	0.83297 (6)	0.0220 (3)
H16A	1.139346	0.021678	0.864745	0.026*
H16B	1.144345	0.072702	0.805811	0.026*
C17	1.02277 (12)	−0.01005 (7)	0.79499 (6)	0.0194 (3)
C18	0.94292 (12)	0.00932 (7)	0.74732 (6)	0.0205 (3)
H18	0.928300	0.057937	0.738951	0.025*
C19	0.88501 (12)	−0.04227 (8)	0.71223 (6)	0.0253 (3)
H19	0.831707	−0.028868	0.679570	0.030*
C20	0.90486 (14)	−0.11361 (8)	0.72479 (7)	0.0314 (3)

H20	0.863894	−0.148864	0.701293	0.038*
C21	0.98439 (15)	−0.13301 (8)	0.77157 (7)	0.0320 (3)
H21	0.998734	−0.181666	0.779895	0.038*
C22	1.04355 (13)	−0.08133 (7)	0.80652 (7)	0.0256 (3)
H22	1.098428	−0.094963	0.838439	0.031*
N1	0.14580 (10)	0.02040 (6)	0.63731 (5)	0.0199 (2)
N2	0.03241 (10)	0.10849 (6)	0.60977 (5)	0.0190 (2)
N3	0.89775 (10)	0.18811 (6)	0.88402 (5)	0.0229 (2)
N4	1.00287 (10)	0.09437 (6)	0.86338 (5)	0.0196 (2)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02669 (8)	0.02857 (8)	0.02379 (7)	−0.00178 (6)	−0.00049 (5)	−0.00815 (5)
Br2	0.02648 (7)	0.02405 (7)	0.02380 (7)	−0.00402 (6)	0.00081 (5)	0.00084 (5)
C1	0.0192 (6)	0.0264 (7)	0.0175 (6)	−0.0047 (5)	0.0002 (5)	0.0005 (5)
C2	0.0216 (6)	0.0225 (7)	0.0175 (6)	−0.0051 (5)	0.0006 (5)	−0.0012 (5)
C3	0.0212 (6)	0.0213 (7)	0.0186 (6)	−0.0025 (5)	0.0009 (5)	−0.0004 (5)
C4	0.0297 (7)	0.0229 (7)	0.0331 (7)	0.0038 (6)	−0.0004 (6)	0.0018 (6)
C5	0.0206 (6)	0.0235 (7)	0.0243 (6)	0.0001 (5)	−0.0023 (5)	0.0022 (5)
C6	0.0197 (6)	0.0223 (7)	0.0221 (6)	0.0010 (5)	−0.0044 (5)	0.0034 (5)
C7	0.0272 (7)	0.0255 (7)	0.0286 (7)	0.0018 (6)	−0.0040 (6)	−0.0005 (6)
C8	0.0321 (8)	0.0213 (7)	0.0477 (9)	−0.0010 (6)	−0.0119 (7)	0.0043 (7)
C9	0.0231 (7)	0.0342 (9)	0.0473 (9)	−0.0041 (6)	−0.0090 (6)	0.0203 (7)
C10	0.0211 (7)	0.0478 (10)	0.0307 (7)	0.0035 (6)	0.0009 (6)	0.0150 (7)
C11	0.0237 (7)	0.0298 (8)	0.0246 (6)	0.0051 (6)	−0.0013 (5)	0.0022 (6)
C12	0.0204 (6)	0.0349 (8)	0.0190 (6)	−0.0056 (6)	0.0010 (5)	−0.0042 (5)
C13	0.0241 (7)	0.0272 (7)	0.0179 (6)	−0.0067 (6)	0.0010 (5)	0.0009 (5)
C14	0.0229 (6)	0.0222 (7)	0.0197 (6)	−0.0023 (5)	0.0010 (5)	−0.0004 (5)
C15	0.0351 (8)	0.0265 (8)	0.0365 (8)	0.0071 (7)	−0.0044 (6)	−0.0079 (6)
C16	0.0194 (6)	0.0239 (7)	0.0227 (6)	0.0021 (5)	0.0003 (5)	−0.0008 (5)
C17	0.0176 (6)	0.0203 (6)	0.0203 (6)	0.0003 (5)	0.0042 (5)	0.0007 (5)
C18	0.0184 (6)	0.0212 (6)	0.0218 (6)	0.0016 (5)	0.0036 (5)	0.0026 (5)
C19	0.0198 (6)	0.0322 (8)	0.0240 (6)	−0.0006 (6)	0.0008 (5)	−0.0007 (6)
C20	0.0319 (8)	0.0272 (8)	0.0350 (8)	−0.0043 (6)	0.0039 (6)	−0.0095 (6)
C21	0.0377 (8)	0.0179 (7)	0.0404 (8)	0.0030 (6)	0.0052 (7)	0.0011 (6)
C22	0.0267 (7)	0.0230 (7)	0.0273 (6)	0.0038 (6)	0.0013 (6)	0.0056 (5)
N1	0.0195 (5)	0.0213 (6)	0.0189 (5)	−0.0012 (4)	0.0014 (4)	0.0008 (4)
N2	0.0191 (5)	0.0202 (6)	0.0176 (5)	−0.0021 (4)	−0.0005 (4)	0.0004 (4)
N3	0.0212 (5)	0.0249 (6)	0.0226 (5)	−0.0005 (5)	−0.0004 (4)	−0.0050 (5)
N4	0.0195 (5)	0.0216 (6)	0.0178 (5)	−0.0015 (4)	0.0004 (4)	−0.0007 (4)

Geometric parameters ($\text{\AA}$, $^\circ$)

C1—C2	1.3504 (19)	C12—C13	1.347 (2)
C1—N1	1.3767 (17)	C12—N3	1.3747 (18)
C1—H1	0.9500	C12—H12	0.9500
C2—N2	1.3820 (16)	C13—N4	1.3819 (16)

C2—H2	0.9500	C13—H13	0.9500
C3—N2	1.3291 (17)	C14—N4	1.3293 (17)
C3—N1	1.3298 (16)	C14—N3	1.3307 (17)
C3—H3	0.9500	C14—H14	0.9500
C4—N1	1.4636 (18)	C15—N3	1.4643 (19)
C4—H4A	0.9800	C15—H15A	0.9800
C4—H4B	0.9800	C15—H15B	0.9800
C4—H4C	0.9800	C15—H15C	0.9800
C5—N2	1.4771 (17)	C16—N4	1.4717 (17)
C5—C6	1.5115 (19)	C16—C17	1.5144 (18)
C5—H5A	0.9900	C16—H16A	0.9900
C5—H5B	0.9900	C16—H16B	0.9900
C6—C7	1.3871 (19)	C17—C22	1.3887 (19)
C6—C11	1.3943 (19)	C17—C18	1.3995 (18)
C7—C8	1.390 (2)	C18—C19	1.388 (2)
C7—H7	0.9500	C18—H18	0.9500
C8—C9	1.383 (2)	C19—C20	1.392 (2)
C8—H8	0.9500	C19—H19	0.9500
C9—C10	1.388 (2)	C20—C21	1.383 (2)
C9—H9	0.9500	C20—H20	0.9500
C10—C11	1.394 (2)	C21—C22	1.394 (2)
C10—H10	0.9500	C21—H21	0.9500
C11—H11	0.9500	C22—H22	0.9500
C2—C1—N1	107.28 (11)	N4—C14—N3	108.38 (12)
C2—C1—H1	126.4	N4—C14—H14	125.8
N1—C1—H1	126.4	N3—C14—H14	125.8
C1—C2—N2	106.76 (12)	N3—C15—H15A	109.5
C1—C2—H2	126.6	N3—C15—H15B	109.5
N2—C2—H2	126.6	H15A—C15—H15B	109.5
N2—C3—N1	108.50 (11)	N3—C15—H15C	109.5
N2—C3—H3	125.7	H15A—C15—H15C	109.5
N1—C3—H3	125.7	H15B—C15—H15C	109.5
N1—C4—H4A	109.5	N4—C16—C17	112.10 (10)
N1—C4—H4B	109.5	N4—C16—H16A	109.2
H4A—C4—H4B	109.5	C17—C16—H16A	109.2
N1—C4—H4C	109.5	N4—C16—H16B	109.2
H4A—C4—H4C	109.5	C17—C16—H16B	109.2
H4B—C4—H4C	109.5	H16A—C16—H16B	107.9
N2—C5—C6	110.22 (11)	C22—C17—C18	119.21 (13)
N2—C5—H5A	109.6	C22—C17—C16	119.76 (12)
C6—C5—H5A	109.6	C18—C17—C16	121.01 (12)
N2—C5—H5B	109.6	C19—C18—C17	120.22 (13)
C6—C5—H5B	109.6	C19—C18—H18	119.9
H5A—C5—H5B	108.1	C17—C18—H18	119.9
C7—C6—C11	119.62 (13)	C18—C19—C20	120.15 (13)
C7—C6—C5	119.66 (12)	C18—C19—H19	119.9
C11—C6—C5	120.70 (13)	C20—C19—H19	119.9

C6—C7—C8	120.26 (14)	C21—C20—C19	119.82 (14)
C6—C7—H7	119.9	C21—C20—H20	120.1
C8—C7—H7	119.9	C19—C20—H20	120.1
C9—C8—C7	120.18 (15)	C20—C21—C22	120.15 (14)
C9—C8—H8	119.9	C20—C21—H21	119.9
C7—C8—H8	119.9	C22—C21—H21	119.9
C8—C9—C10	119.95 (14)	C17—C22—C21	120.42 (13)
C8—C9—H9	120.0	C17—C22—H22	119.8
C10—C9—H9	120.0	C21—C22—H22	119.8
C9—C10—C11	120.09 (14)	C3—N1—C1	108.69 (11)
C9—C10—H10	120.0	C3—N1—C4	124.92 (12)
C11—C10—H10	120.0	C1—N1—C4	126.38 (11)
C10—C11—C6	119.89 (14)	C3—N2—C2	108.76 (11)
C10—C11—H11	120.1	C3—N2—C5	125.20 (11)
C6—C11—H11	120.1	C2—N2—C5	125.92 (11)
C13—C12—N3	107.33 (12)	C14—N3—C12	108.73 (12)
C13—C12—H12	126.3	C14—N3—C15	124.82 (12)
N3—C12—H12	126.3	C12—N3—C15	126.45 (12)
C12—C13—N4	106.84 (12)	C14—N4—C13	108.72 (11)
C12—C13—H13	126.6	C14—N4—C16	125.44 (11)
N4—C13—H13	126.6	C13—N4—C16	125.83 (12)
N1—C1—C2—N2	−0.17 (14)	C20—C21—C22—C17	0.4 (2)
N2—C5—C6—C7	−103.83 (14)	N2—C3—N1—C1	−0.01 (14)
N2—C5—C6—C11	74.65 (15)	N2—C3—N1—C4	178.70 (12)
C11—C6—C7—C8	−0.2 (2)	C2—C1—N1—C3	0.12 (14)
C5—C6—C7—C8	178.27 (13)	C2—C1—N1—C4	−178.57 (12)
C6—C7—C8—C9	0.2 (2)	N1—C3—N2—C2	−0.10 (14)
C7—C8—C9—C10	0.2 (2)	N1—C3—N2—C5	176.21 (11)
C8—C9—C10—C11	−0.5 (2)	C1—C2—N2—C3	0.17 (14)
C9—C10—C11—C6	0.4 (2)	C1—C2—N2—C5	−176.11 (12)
C7—C6—C11—C10	−0.1 (2)	C6—C5—N2—C3	−116.36 (14)
C5—C6—C11—C10	−178.54 (12)	C6—C5—N2—C2	59.32 (16)
N3—C12—C13—N4	−0.04 (15)	N4—C14—N3—C12	0.03 (15)
N4—C16—C17—C22	−123.69 (13)	N4—C14—N3—C15	−179.51 (12)
N4—C16—C17—C18	57.74 (16)	C13—C12—N3—C14	0.01 (15)
C22—C17—C18—C19	0.23 (19)	C13—C12—N3—C15	179.54 (13)
C16—C17—C18—C19	178.81 (12)	N3—C14—N4—C13	−0.05 (14)
C17—C18—C19—C20	0.8 (2)	N3—C14—N4—C16	179.45 (11)
C18—C19—C20—C21	−1.3 (2)	C12—C13—N4—C14	0.06 (15)
C19—C20—C21—C22	0.7 (2)	C12—C13—N4—C16	−179.44 (12)
C18—C17—C22—C21	−0.8 (2)	C17—C16—N4—C14	−105.12 (14)
C16—C17—C22—C21	−179.41 (13)	C17—C16—N4—C13	74.30 (15)