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1,4-Dimethylpyridinium iodide

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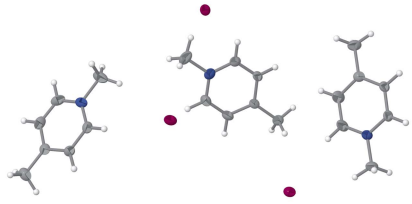
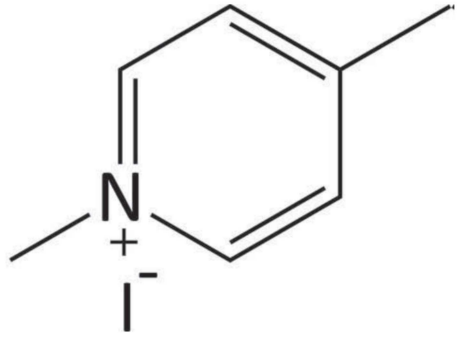
Structural data: full structural data are available from iucrdata.iucr.org

The title organic salt, $C_7H_{10}N^+\cdot I^-$, was synthesized from a mixture of 4-methylpyridine and iodomethane in 2-propanol. It crystallized with three independent 1,4-dimethylpyridinium cations and three independent iodide anions in the asymmetric unit. In the crystal, there are no significant intermolecular interactions present.

3D view



Chemical scheme



Structure description

The title organic salt was synthesized from a mixture of 4-methylpyridine and iodomethane in 2-propanol. It crystallized with three independent 1,4-dimethylpyridinium cations and three independent iodide anions in the asymmetric unit (Fig. 1). In the crystal (Fig. 2), there are no significant intermolecular interactions present. The H···I distances vary between *ca* 3.06 and 3.16 Å.

The crystal structures of the triiodide (Tan *et al.*, 2005) and the heptaiodide (Herbstein *et al.*, 1985) salts of 1,4-dimethylpyridinium have been reported.

Synthesis and crystallization

The title molecular salt was synthesized (Ault, 1997) from a mixture of 4-methylpyridine (0.10 mol, 10.0 mL) and iodomethane (0.10 mol, 6.2 mL) in 2-propanol (20 mL) (Fig. 3). The solution was heated to 323 K using a water bath to initiate the reaction. Upon reaching 323 K, the solution was removed from the water bath and allowed to cool to room temperature. After 30 min, the colorless block-like crystals that formed were collected by vacuum filtration (yield: 21.0 g, 89%).

Refinement

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

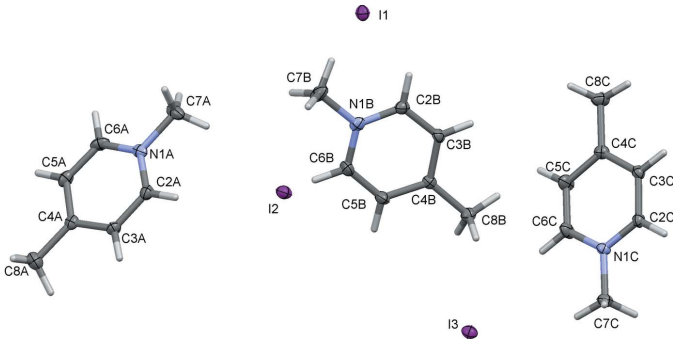


Figure 1
A view of the molecular structure of the title compound, showing the atom labeling and 50% probability displacement ellipsoids.

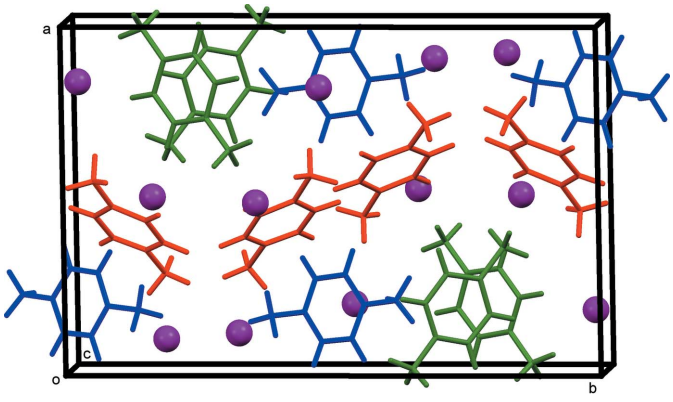


Figure 2
A view along the *c* axis of the crystal packing of the title compound (color code: I^- = violet balls, cation *A* = blue, cation *B* = red, and cation *C* = green).

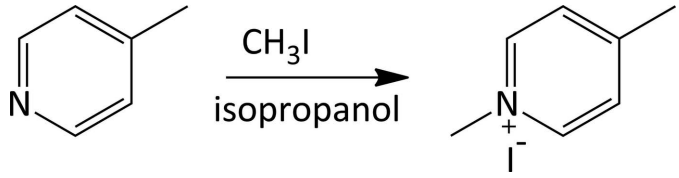


Figure 3
Synthesis of the title organic salt.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_7H_{10}N^+\cdot I^-$
M_r	235.06
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	13.8301 (6), 19.7170 (9), 10.2121 (5)
β (°)	109.642 (1)
V (Å^3)	2622.7 (2)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.59
Crystal size (mm)	0.5 × 0.5 × 0.3
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.476, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16106, 5933, 5401
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.658
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.021, 0.048, 1.14
No. of reflections	5933
No. of parameters	251
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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full crystallographic data

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Crystal data

$C_7H_{10}N^+·I^-$
M_r = 235.06
Monoclinic, $P2_1/c$
a = 13.8301 (6) Å
b = 19.7170 (9) Å
c = 10.2121 (5) Å
β = 109.642 (1)°
V = 2622.7 (2) Å^3
Z = 12
$F(000)$ = 1344
D_x = 1.786 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9919 reflections
θ = 3.0–27.9°
μ = 3.59 mm^{-1}
T = 150 K
Block, clear colourless
0.5 × 0.5 × 0.3 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.476, T_{max} = 0.746
16106 measured reflections
5933 independent reflections
5401 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.9°, θ_{min} = 3.0°
h = −18→16
k = −25→22
l = −10→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.048
S = 1.14
5933 reflections
251 parameters
0 restraints
Primary atom site location: heavy-atom method
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.013P)^2 + 2.567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: (SHELXL2014; Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00371 (9)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1A	0.17247 (17)	0.06045 (10)	0.8272 (2)	0.0280 (4)
C2A	0.26459 (19)	0.04078 (13)	0.9118 (3)	0.0293 (5)
H2A	0.3244	0.0639	0.9101	0.035*
C3A	0.27371 (19)	−0.01251 (13)	1.0013 (3)	0.0282 (5)
H3A	0.3399	−0.0261	1.0603	0.034*
C4A	0.18709 (19)	−0.04710 (12)	1.0073 (3)	0.0254 (5)
C5A	0.09273 (19)	−0.02508 (13)	0.9167 (3)	0.0323 (6)
H5A	0.0316	−0.0474	0.9156	0.039*
C6A	0.0873 (2)	0.02837 (14)	0.8291 (3)	0.0343 (6)
H6A	0.0221	0.0431	0.7686	0.041*
C7A	0.1643 (3)	0.11948 (14)	0.7343 (3)	0.0425 (7)
H7AA	0.2303	0.1269	0.7208	0.064*
H7AB	0.1458	0.1599	0.7765	0.064*
H7AC	0.1112	0.1107	0.6443	0.064*
C8A	0.1962 (2)	−0.10450 (14)	1.1067 (3)	0.0385 (6)
H8AA	0.1373	−0.1350	1.0699	0.058*
H8AB	0.1974	−0.0865	1.1967	0.058*
H8AC	0.2597	−0.1296	1.1187	0.058*
N1B	0.34851 (16)	0.14589 (11)	0.3646 (2)	0.0282 (4)
C2B	0.37389 (18)	0.17934 (12)	0.2661 (3)	0.0282 (5)
H2B	0.3472	0.2235	0.2388	0.034*
C3B	0.43849 (18)	0.15008 (12)	0.2045 (3)	0.0265 (5)
H3B	0.4561	0.1743	0.1353	0.032*
C4B	0.47783 (18)	0.08550 (11)	0.2429 (2)	0.0228 (5)
C5B	0.4466 (2)	0.05136 (13)	0.3414 (3)	0.0320 (6)
H5B	0.4693	0.0062	0.3669	0.038*
C6B	0.3831 (2)	0.08253 (14)	0.4018 (3)	0.0351 (6)
H6B	0.3636	0.0592	0.4704	0.042*
C7B	0.2809 (2)	0.17861 (17)	0.4316 (3)	0.0432 (7)
H7BA	0.2236	0.1483	0.4262	0.065*
H7BB	0.2542	0.2212	0.3837	0.065*
H7BC	0.3202	0.1880	0.5293	0.065*
C8B	0.5518 (2)	0.05338 (13)	0.1828 (3)	0.0299 (5)
H8BA	0.5324	0.0059	0.1595	0.045*
H8BB	0.6213	0.0554	0.2510	0.045*
H8BC	0.5501	0.0779	0.0985	0.045*
N1C	0.89692 (15)	0.18673 (9)	0.2697 (2)	0.0235 (4)
C2C	0.91494 (19)	0.24514 (12)	0.2131 (3)	0.0261 (5)
H2C	0.9836	0.2584	0.2264	0.031*
C3C	0.83548 (19)	0.28570 (12)	0.1369 (3)	0.0260 (5)
H3C	0.8496	0.3266	0.0977	0.031*
C4C	0.73442 (19)	0.26743 (12)	0.1164 (3)	0.0258 (5)
C5C	0.7189 (2)	0.20670 (15)	0.1763 (3)	0.0397 (7)
H5C	0.6509	0.1923	0.1642	0.048*
C6C	0.8000 (2)	0.16742 (14)	0.2523 (3)	0.0348 (6)

H6C	0.7878	0.1264	0.2929	0.042*
C7C	0.9849 (2)	0.14490 (13)	0.3522 (3)	0.0309 (5)
H7CA	0.9597	0.1042	0.3854	0.046*
H7CB	1.0280	0.1712	0.4320	0.046*
H7CC	1.0255	0.1316	0.2940	0.046*
C8C	0.6457 (2)	0.31053 (14)	0.0333 (3)	0.0365 (6)
H8CA	0.6045	0.3231	0.0911	0.055*
H8CB	0.6030	0.2850	−0.0479	0.055*
H8CC	0.6715	0.3517	0.0024	0.055*
I1	0.10438 (2)	0.18819 (2)	0.05002 (2)	0.02898 (5)
I2	0.48598 (2)	0.14790 (2)	0.80737 (2)	0.03174 (5)
I3	0.82578 (2)	0.01901 (2)	0.52125 (2)	0.02898 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1A	0.0402 (12)	0.0249 (10)	0.0194 (10)	0.0074 (9)	0.0107 (10)	−0.0014 (8)
C2A	0.0261 (12)	0.0309 (12)	0.0334 (14)	−0.0016 (10)	0.0133 (11)	−0.0008 (10)
C3A	0.0203 (11)	0.0326 (13)	0.0291 (13)	0.0001 (9)	0.0049 (11)	0.0024 (10)
C4A	0.0277 (12)	0.0249 (11)	0.0243 (12)	−0.0017 (9)	0.0097 (11)	−0.0063 (9)
C5A	0.0222 (12)	0.0360 (14)	0.0376 (15)	−0.0056 (10)	0.0088 (12)	−0.0090 (11)
C6A	0.0251 (12)	0.0395 (14)	0.0298 (14)	0.0071 (10)	−0.0021 (12)	−0.0059 (11)
C7A	0.070 (2)	0.0321 (14)	0.0283 (14)	0.0153 (14)	0.0203 (15)	0.0070 (11)
C8A	0.0462 (17)	0.0357 (14)	0.0347 (14)	−0.0042 (12)	0.0151 (14)	0.0045 (11)
N1B	0.0221 (10)	0.0379 (12)	0.0217 (10)	0.0014 (8)	0.0036 (9)	−0.0037 (8)
C2B	0.0226 (11)	0.0247 (12)	0.0354 (14)	−0.0015 (9)	0.0072 (11)	0.0010 (10)
C3B	0.0233 (11)	0.0236 (11)	0.0321 (13)	−0.0038 (9)	0.0088 (11)	0.0060 (9)
C4B	0.0222 (11)	0.0227 (11)	0.0197 (11)	−0.0042 (8)	0.0020 (10)	−0.0017 (8)
C5B	0.0381 (14)	0.0269 (12)	0.0308 (13)	0.0049 (10)	0.0113 (12)	0.0085 (10)
C6B	0.0377 (15)	0.0409 (15)	0.0284 (13)	0.0040 (11)	0.0132 (13)	0.0112 (11)
C7B	0.0339 (15)	0.068 (2)	0.0291 (14)	0.0137 (14)	0.0118 (13)	−0.0059 (13)
C8B	0.0298 (12)	0.0278 (12)	0.0321 (13)	0.0022 (10)	0.0102 (11)	−0.0001 (10)
N1C	0.0248 (10)	0.0216 (9)	0.0220 (10)	−0.0003 (7)	0.0050 (9)	0.0002 (7)
C2C	0.0267 (12)	0.0240 (11)	0.0299 (12)	−0.0033 (9)	0.0124 (11)	0.0010 (9)
C3C	0.0295 (12)	0.0220 (11)	0.0276 (12)	−0.0015 (9)	0.0110 (11)	0.0023 (9)
C4C	0.0264 (12)	0.0247 (11)	0.0237 (12)	−0.0003 (9)	0.0051 (10)	−0.0026 (9)
C5C	0.0230 (12)	0.0405 (15)	0.0497 (18)	−0.0088 (11)	0.0044 (13)	0.0111 (13)
C6C	0.0273 (13)	0.0316 (13)	0.0406 (15)	−0.0098 (10)	0.0049 (12)	0.0105 (11)
C7C	0.0270 (12)	0.0280 (12)	0.0332 (14)	0.0030 (10)	0.0042 (11)	0.0055 (10)
C8C	0.0286 (13)	0.0349 (14)	0.0394 (15)	0.0040 (11)	0.0026 (13)	0.0035 (11)
I1	0.03136 (9)	0.03198 (9)	0.02415 (9)	−0.00129 (6)	0.01007 (7)	−0.00118 (6)
I2	0.03101 (9)	0.02680 (9)	0.03405 (10)	0.00249 (6)	0.00652 (8)	0.00621 (6)
I3	0.03280 (9)	0.02248 (8)	0.02966 (9)	0.00116 (6)	0.00787 (7)	−0.00018 (6)

Geometric parameters (Å, º)

N1A—C2A	1.334 (3)	C5B—H5B	0.9500
N1A—C6A	1.343 (4)	C5B—C6B	1.376 (4)

N1A—C7A	1.481 (3)	C6B—H6B	0.9500
C2A—H2A	0.9500	C7B—H7BA	0.9800
C2A—C3A	1.370 (4)	C7B—H7BB	0.9800
C3A—H3A	0.9500	C7B—H7BC	0.9800
C3A—C4A	1.397 (3)	C8B—H8BA	0.9800
C4A—C5A	1.391 (4)	C8B—H8BB	0.9800
C4A—C8A	1.498 (4)	C8B—H8BC	0.9800
C5A—H5A	0.9500	N1C—C2C	1.349 (3)
C5A—C6A	1.368 (4)	N1C—C6C	1.347 (3)
C6A—H6A	0.9500	N1C—C7C	1.477 (3)
C7A—H7AA	0.9800	C2C—H2C	0.9500
C7A—H7AB	0.9800	C2C—C3C	1.371 (3)
C7A—H7AC	0.9800	C3C—H3C	0.9500
C8A—H8AA	0.9800	C3C—C4C	1.389 (3)
C8A—H8AB	0.9800	C4C—C5C	1.394 (4)
C8A—H8AC	0.9800	C4C—C8C	1.500 (3)
N1B—C2B	1.344 (3)	C5C—H5C	0.9500
N1B—C6B	1.346 (3)	C5C—C6C	1.369 (4)
N1B—C7B	1.480 (3)	C6C—H6C	0.9500
C2B—H2B	0.9500	C7C—H7CA	0.9800
C2B—C3B	1.381 (4)	C7C—H7CB	0.9800
C3B—H3B	0.9500	C7C—H7CC	0.9800
C3B—C4B	1.389 (3)	C8C—H8CA	0.9800
C4B—C5B	1.394 (3)	C8C—H8CB	0.9800
C4B—C8B	1.499 (3)	C8C—H8CC	0.9800

C2A—N1A—C6A	120.3 (2)	N1B—C6B—C5B	120.5 (2)
C2A—N1A—C7A	119.6 (2)	N1B—C6B—H6B	119.7
C6A—N1A—C7A	120.0 (2)	C5B—C6B—H6B	119.7
N1A—C2A—H2A	119.7	N1B—C7B—H7BA	109.5
N1A—C2A—C3A	120.6 (2)	N1B—C7B—H7BB	109.5
C3A—C2A—H2A	119.7	N1B—C7B—H7BC	109.5
C2A—C3A—H3A	119.5	H7BA—C7B—H7BB	109.5
C2A—C3A—C4A	121.0 (2)	H7BA—C7B—H7BC	109.5
C4A—C3A—H3A	119.5	H7BB—C7B—H7BC	109.5
C3A—C4A—C8A	121.4 (2)	C4B—C8B—H8BA	109.5
C5A—C4A—C3A	116.4 (2)	C4B—C8B—H8BB	109.5
C5A—C4A—C8A	122.2 (2)	C4B—C8B—H8BC	109.5
C4A—C5A—H5A	119.7	H8BA—C8B—H8BB	109.5
C6A—C5A—C4A	120.6 (2)	H8BA—C8B—H8BC	109.5
C6A—C5A—H5A	119.7	H8BB—C8B—H8BC	109.5
N1A—C6A—C5A	121.1 (2)	C2C—N1C—C7C	119.0 (2)
N1A—C6A—H6A	119.5	C6C—N1C—C2C	120.3 (2)
C5A—C6A—H6A	119.5	C6C—N1C—C7C	120.7 (2)
N1A—C7A—H7AA	109.5	N1C—C2C—H2C	119.6
N1A—C7A—H7AB	109.5	N1C—C2C—C3C	120.9 (2)
N1A—C7A—H7AC	109.5	C3C—C2C—H2C	119.6
H7AA—C7A—H7AB	109.5	C2C—C3C—H3C	119.7

H7AA—C7A—H7AC	109.5	C2C—C3C—C4C	120.5 (2)
H7AB—C7A—H7AC	109.5	C4C—C3C—H3C	119.7
C4A—C8A—H8AA	109.5	C3C—C4C—C5C	116.9 (2)
C4A—C8A—H8AB	109.5	C3C—C4C—C8C	121.9 (2)
C4A—C8A—H8AC	109.5	C5C—C4C—C8C	121.2 (2)
H8AA—C8A—H8AB	109.5	C4C—C5C—H5C	119.4
H8AA—C8A—H8AC	109.5	C6C—C5C—C4C	121.2 (2)
H8AB—C8A—H8AC	109.5	C6C—C5C—H5C	119.4
C2B—N1B—C6B	120.6 (2)	N1C—C6C—C5C	120.3 (2)
C2B—N1B—C7B	119.8 (2)	N1C—C6C—H6C	119.9
C6B—N1B—C7B	119.6 (2)	C5C—C6C—H6C	119.9
N1B—C2B—H2B	119.7	N1C—C7C—H7CA	109.5
N1B—C2B—C3B	120.5 (2)	N1C—C7C—H7CB	109.5
C3B—C2B—H2B	119.7	N1C—C7C—H7CC	109.5
C2B—C3B—H3B	119.8	H7CA—C7C—H7CB	109.5
C2B—C3B—C4B	120.4 (2)	H7CA—C7C—H7CC	109.5
C4B—C3B—H3B	119.8	H7CB—C7C—H7CC	109.5
C3B—C4B—C5B	117.4 (2)	C4C—C8C—H8CA	109.5
C3B—C4B—C8B	121.9 (2)	C4C—C8C—H8CB	109.5
C5B—C4B—C8B	120.7 (2)	C4C—C8C—H8CC	109.5
C4B—C5B—H5B	119.8	H8CA—C8C—H8CB	109.5
C6B—C5B—C4B	120.5 (2)	H8CA—C8C—H8CC	109.5
C6B—C5B—H5B	119.8	H8CB—C8C—H8CC	109.5

N1A—C2A—C3A—C4A	−0.6 (4)	C4B—C5B—C6B—N1B	1.5 (4)
C2A—N1A—C6A—C5A	−0.4 (4)	C6B—N1B—C2B—C3B	−2.0 (4)
C2A—C3A—C4A—C5A	0.9 (4)	C7B—N1B—C2B—C3B	178.7 (2)
C2A—C3A—C4A—C8A	−178.8 (2)	C7B—N1B—C6B—C5B	−179.6 (3)
C3A—C4A—C5A—C6A	−0.9 (4)	C8B—C4B—C5B—C6B	176.4 (2)
C4A—C5A—C6A—N1A	0.7 (4)	N1C—C2C—C3C—C4C	0.1 (4)
C6A—N1A—C2A—C3A	0.3 (4)	C2C—N1C—C6C—C5C	0.4 (4)
C7A—N1A—C2A—C3A	178.2 (2)	C2C—C3C—C4C—C5C	−0.1 (4)
C7A—N1A—C6A—C5A	−178.2 (2)	C2C—C3C—C4C—C8C	−179.9 (2)
C8A—C4A—C5A—C6A	178.7 (3)	C3C—C4C—C5C—C6C	0.3 (4)
N1B—C2B—C3B—C4B	0.3 (4)	C4C—C5C—C6C—N1C	−0.5 (5)
C2B—N1B—C6B—C5B	1.1 (4)	C6C—N1C—C2C—C3C	−0.2 (4)
C2B—C3B—C4B—C5B	2.2 (4)	C7C—N1C—C2C—C3C	−179.4 (2)
C2B—C3B—C4B—C8B	−177.2 (2)	C7C—N1C—C6C—C5C	179.6 (3)
C3B—C4B—C5B—C6B	−3.0 (4)	C8C—C4C—C5C—C6C	−179.9 (3)