

Crystal structure of *catena*-poly[1,3-dibenzylbenzimidazolium [[chlorido-mercurate(II)]-di- μ -chlorido]]

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The asymmetric unit of the polymeric title compound, $\{(C_{21}H_{19}N_2)[HgCl_3]\}_n$, comprises one-half of the cationic molecule, the other half being generated by application of twofold rotation symmetry, one Hg and two Cl atoms. The Hg^{II} atom, lying on a twofold rotation axis, exhibits a distorted triangular coordination environment and is surrounded by three Cl atoms with Hg–Cl distances in the range 2.359 (2)–2.4754 (13) Å. Two additional longer distances [Hg...Cl = 3.104 (14) Å] lead to the formation of polymeric $[HgCl_{1/1}Cl_{4/2}]^-$ chains extending along [001]. The crystal packing can be described by cationic layers alternating parallel to $(\bar{1}10)$ with the anionic chains located between the layers. The packing is consolidated by π – π stacking interactions between the benzene rings of the central benzimidazole entities, with centroid-to-centroid distances of 3.643 (3) Å.

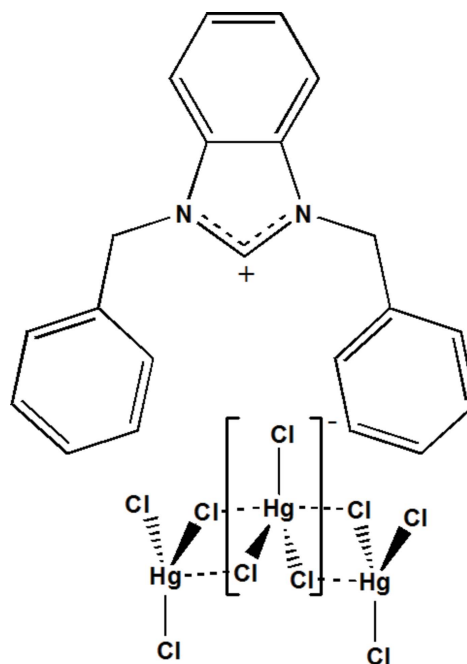
Keywords: crystal structure; benzimidazole derivative; trichlorido-mercurate.

CCDC reference: 1440716

1. Related literature

Benzimidazoles and their derivatives show anti-oxidant (Kuş *et al.*, 2004), antifungal (Preston, 1974) and anthelmintic (Hazelton *et al.*, 1995) properties and have applications in pharmacy and agriculture (Malek *et al.*, 2006). They can also

be used as epoxy resin curing agents, catalysts, metallic surface treatment agents (Li *et al.*, 2003; Abboud *et al.*, 2006) or as ionic liquids (Li *et al.*, 2011; Chen *et al.*, 2008). For the importance of transition metals ions in biological processes, see: Kaim & Schwederski (1994). For bond lengths of delocalized systems, see: Ennajih *et al.* (2009).



2. Experimental

2.1. Crystal data

$(C_{21}H_{19}N_2)[HgCl_3]$
 $M_r = 606.32$
 Monoclinic, $C2/c$
 $a = 20.3669$ (11) Å
 $b = 14.8837$ (7) Å
 $c = 7.2154$ (4) Å
 $\beta = 104.372$ (2)°

$V = 2118.79$ (19) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 7.65$ mm⁻¹
 $T = 295$ K
 $0.19 \times 0.11 \times 0.05$ mm

2.2. Data collection

Bruker APEXII CCD
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2011)
 $T_{min} = 0.646$, $T_{max} = 0.746$

8306 measured reflections
 2401 independent reflections
 1571 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.042$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.085$
 $S = 1.00$
 2401 reflections

124 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 2.02$ e Å⁻³
 $\Delta\rho_{min} = -0.41$ e Å⁻³

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2011); data reduction: SAINT; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and DIAMOND (Bran-

denburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5248).

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supporting information

Acta Cryst. (2015). E71, m255–m256 [<https://doi.org/10.1107/S2056989015023427>]

Crystal structure of *catena*-poly[1,3-dibenzylbenzimidazolium [[chloridomercurate(II)]-di- μ -chlorido]]

**Mehdi Bouchouit, Abdelmalek Bouraiou, Sofiane Bouacida, Hocine Merazig, Ali Belfaitah and
Mebarek Bahnous**

S1. Experimental

1,3-Dibenzylbenzimidazolium trichloridomercurate(II) was synthesized by reaction of 1 mmol of 1,3-dibenzylbenzimidazolium chloride with 1 mmol of mercury(II) chloride in methanol at room temperature. The solid obtained was recrystallized in methanol to yield yellow crystals of the title compound suitable for X-ray diffraction.

S2. Refinement

H atoms were localized from difference maps but were modelled in calculated positions and treated as riding on their parent atom with C—H = 0.93 Å (aromatic), C—H = 0.97 Å (methylene) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{aromatic}} \text{ or } \text{C}_{\text{methylene}})$.

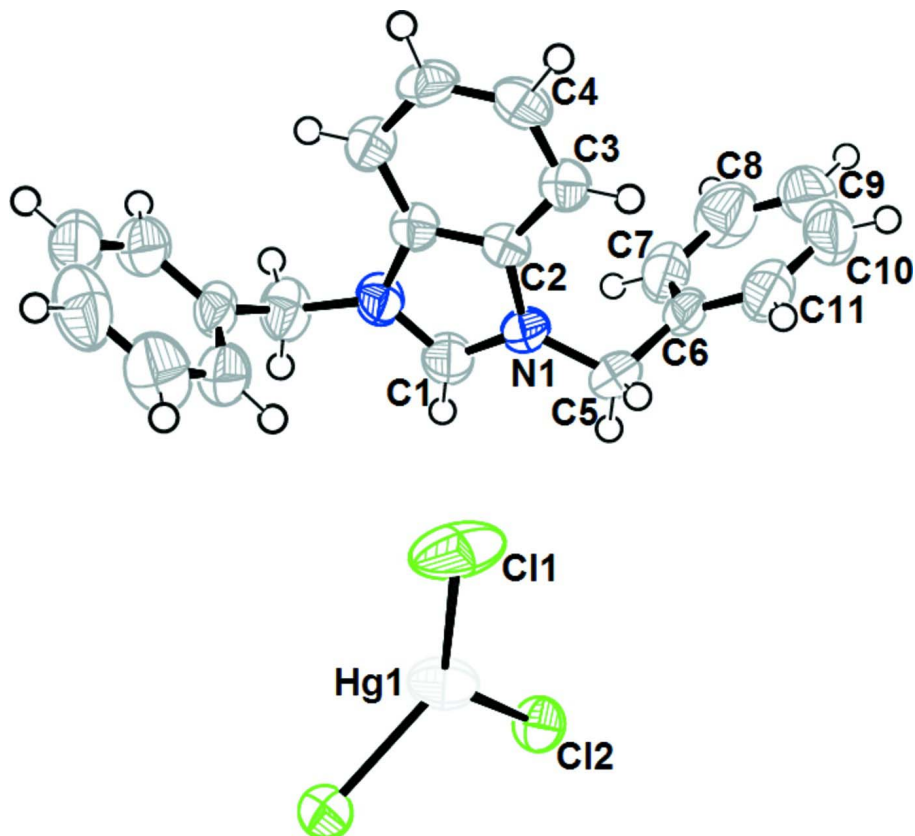


Figure 1

The molecular structures of the entities in the title compound. Displacement ellipsoids are drawn at the 50% probability level; H atoms are represented as small spheres of arbitrary radius. Non-labelled atoms are generated by symmetry code $2 - x, y, 3/2 - z$ for the cation and by symmetry code $2 - x, y, 1/2 - z$ for the anion.

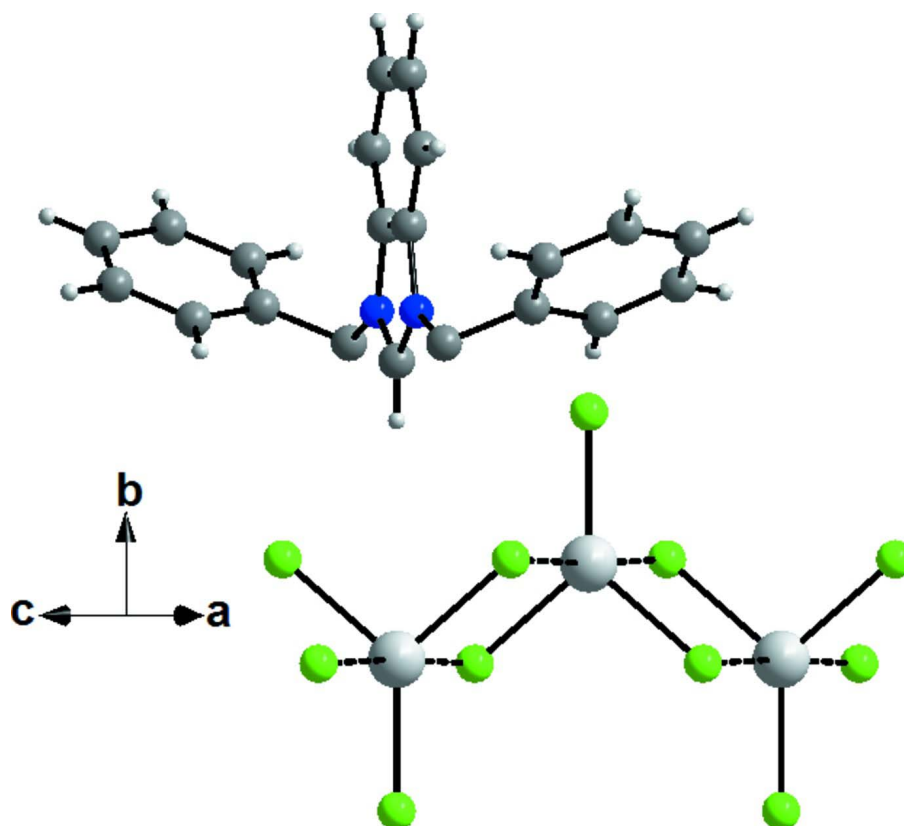


Figure 2

The polymeric anionic $[\text{HgCl}_{1/1}\text{Cl}_{4/2}]^{-}$ chain defined by long Hg—Cl distances (in dashed lines).

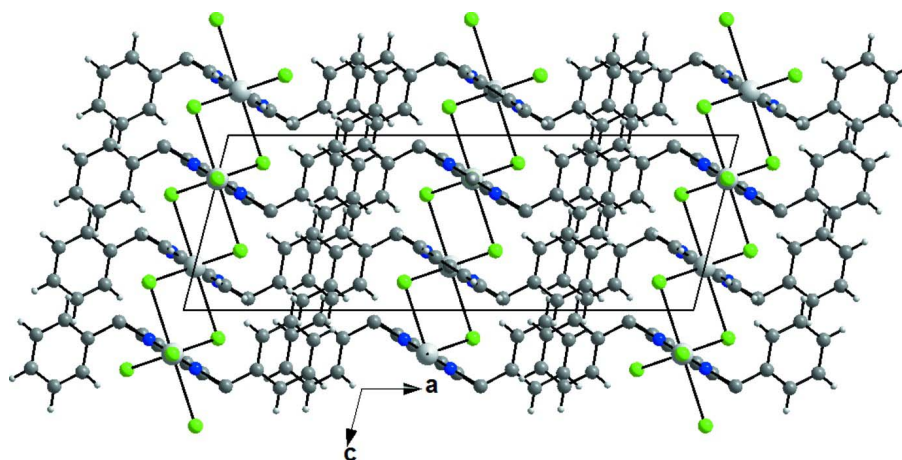


Figure 3

The crystal packing of the title compound viewed down $[010]$ showing alternating layers of cations and anions.

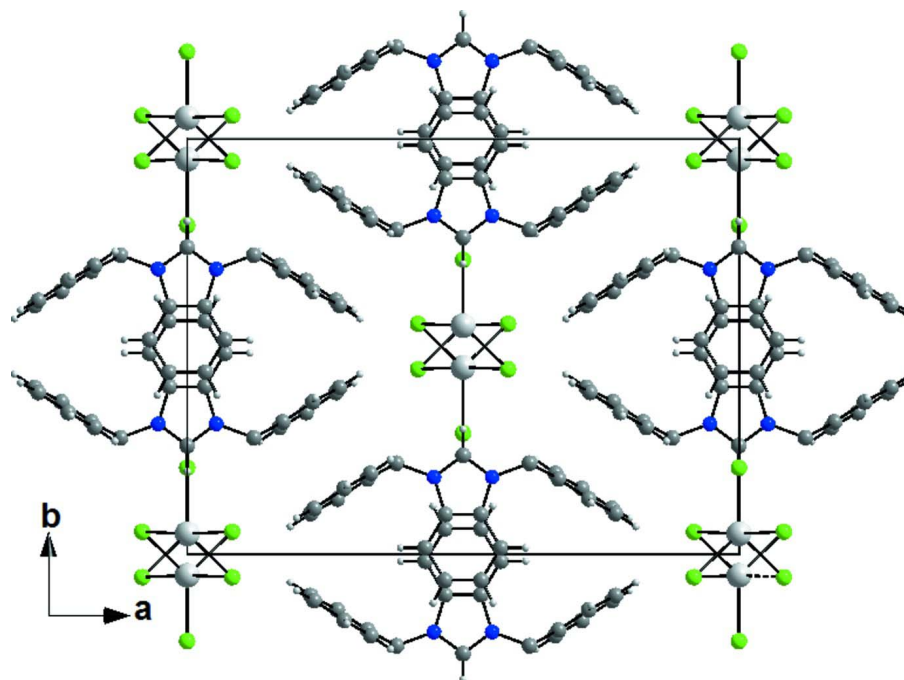


Figure 4

The crystal packing of the title compound viewed down [001] (chain direction).

catena-Poly[1,3-dibenzylbenzimidazolium [[chloridomercurate(II)]-di- μ -chlorido]]

Crystal data

(C₂₁H₁₉N₂)[HgCl₃]

$M_r = 606.32$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 20.3669$ (11) Å

$b = 14.8837$ (7) Å

$c = 7.2154$ (4) Å

$\beta = 104.372$ (2)°

$V = 2118.79$ (19) Å³

$Z = 4$

$F(000) = 1160$

$D_x = 1.901$ Mg m⁻³

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

Cell parameters from 2352 reflections

$\theta = 2.7$ – 22.8°

$\mu = 7.65$ mm⁻¹

$T = 295$ K

Prism, yellow

$0.19 \times 0.11 \times 0.05$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: Enraf Nonius FR590

Graphite monochromator

CCD rotation images, thick slices scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2011)

$T_{\min} = 0.646$, $T_{\max} = 0.746$

8306 measured reflections

2401 independent reflections

1571 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -26 \rightarrow 26$

$k = -18 \rightarrow 13$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.085$
 $S = 1.00$
 2401 reflections
 124 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
 $w = 1/[\sigma^2(F_o^2) + (0.0419P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 2.02 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.41 \text{ e } \text{Å}^{-3}$

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.

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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	1	0.050020 (19)	0.25	0.05935 (16)
Cl2	0.91850 (7)	-0.05454 (8)	0.33958 (18)	0.0473 (3)
Cl1	1	0.20850 (14)	0.25	0.0888 (9)
N1	0.9472 (2)	0.3140 (3)	0.6672 (6)	0.0415 (10)
C4	1	0.2622 (5)	0.75	0.0484 (19)
H4	1	0.1998	0.75	0.058*
C6	0.8265 (3)	0.3186 (3)	0.6596 (8)	0.0446 (13)
C3	0.9676 (2)	0.4034 (3)	0.6988 (6)	0.0348 (11)
C1	0.9672 (3)	0.5616 (3)	0.6966 (8)	0.0463 (14)
H1	0.9458	0.6165	0.6613	0.056*
C2	0.9314 (3)	0.4838 (4)	0.6393 (7)	0.0418 (12)
H2	0.8868	0.4841	0.5667	0.05*
C5	0.8795 (3)	0.2814 (4)	0.5694 (8)	0.0524 (14)
H5A	0.8789	0.2163	0.5749	0.063*
H5B	0.8694	0.299	0.4359	0.063*
C7	0.8324 (3)	0.3053 (4)	0.8527 (9)	0.0569 (15)
H7	0.8683	0.2721	0.9258	0.068*
C11	0.7722 (3)	0.3668 (4)	0.5561 (9)	0.0574 (15)
H11	0.768	0.3764	0.4263	0.069*
C8	0.7847 (4)	0.3418 (5)	0.9352 (9)	0.0751 (19)
H8	0.7893	0.3342	1.0658	0.09*
C9	0.7303 (3)	0.3891 (5)	0.8308 (12)	0.075 (2)
H9	0.6982	0.4127	0.8894	0.091*
C10	0.7238 (3)	0.4013 (4)	0.6396 (12)	0.0695 (18)
H10	0.6869	0.4327	0.5663	0.083*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0830 (3)	0.02880 (19)	0.0678 (2)	0	0.02171 (18)	0
Cl2	0.0457 (8)	0.0495 (8)	0.0472 (7)	-0.0016 (6)	0.0120 (6)	0.0026 (6)
Cl1	0.146 (3)	0.0298 (12)	0.0719 (15)	0	-0.0079 (15)	0
N1	0.037 (3)	0.031 (2)	0.053 (3)	-0.0031 (19)	0.006 (2)	-0.0073 (19)
C4	0.043 (5)	0.033 (4)	0.068 (5)	0	0.010 (4)	0
C6	0.031 (3)	0.032 (3)	0.064 (4)	-0.005 (2)	-0.002 (3)	-0.008 (2)
C3	0.037 (3)	0.033 (3)	0.036 (3)	0.003 (2)	0.012 (2)	-0.003 (2)
C1	0.055 (3)	0.029 (3)	0.056 (3)	0.011 (2)	0.014 (3)	0.006 (2)
C2	0.039 (3)	0.042 (3)	0.042 (3)	0.003 (2)	0.006 (2)	-0.003 (2)
C5	0.044 (3)	0.048 (3)	0.059 (3)	-0.005 (3)	0.001 (3)	-0.018 (3)
C7	0.042 (4)	0.060 (4)	0.063 (4)	-0.004 (3)	0.001 (3)	0.003 (3)
C11	0.048 (4)	0.056 (4)	0.062 (4)	-0.007 (3)	0.001 (3)	0.002 (3)
C8	0.068 (5)	0.098 (6)	0.062 (4)	-0.013 (4)	0.020 (4)	-0.012 (4)
C9	0.052 (4)	0.075 (5)	0.106 (6)	-0.007 (4)	0.033 (4)	-0.027 (4)
C10	0.043 (4)	0.053 (4)	0.109 (6)	0.000 (3)	0.012 (4)	-0.001 (4)

Geometric parameters (\AA , $^\circ$)

Hg1—Cl1	2.359 (2)	C1—C2	1.376 (7)
Hg1—Cl2 ⁱ	2.4754 (13)	C1—H1	0.93
Hg1—Cl2	2.4754 (13)	C2—H2	0.93
N1—C4	1.336 (6)	C5—H5A	0.97
N1—C3	1.397 (6)	C5—H5B	0.97
N1—C5	1.466 (6)	C7—C8	1.372 (9)
C4—N1 ⁱⁱ	1.336 (6)	C7—H7	0.93
C4—H4	0.93	C11—C10	1.375 (9)
C6—C11	1.374 (7)	C11—H11	0.93
C6—C7	1.383 (8)	C8—C9	1.370 (10)
C6—C5	1.499 (7)	C8—H8	0.93
C3—C3 ⁱⁱ	1.344 (9)	C9—C10	1.365 (10)
C3—C2	1.414 (7)	C9—H9	0.93
C1—C1 ⁱⁱ	1.367 (11)	C10—H10	0.93
Cl1—Hg1—Cl2 ⁱ	128.95 (3)	N1—C5—C6	111.2 (4)
Cl1—Hg1—Cl2	128.95 (3)	N1—C5—H5A	109.4
Cl2 ⁱ —Hg1—Cl2	102.09 (6)	C6—C5—H5A	109.4
C4—N1—C3	107.6 (4)	N1—C5—H5B	109.4
C4—N1—C5	125.5 (4)	C6—C5—H5B	109.4
C3—N1—C5	126.8 (4)	H5A—C5—H5B	108
N1 ⁱⁱ —C4—N1	109.7 (6)	C8—C7—C6	119.1 (6)
N1 ⁱⁱ —C4—H4	125.2	C8—C7—H7	120.4
N1—C4—H4	125.2	C6—C7—H7	120.4
C11—C6—C7	118.7 (6)	C6—C11—C10	121.7 (6)
C11—C6—C5	121.8 (5)	C6—C11—H11	119.2
C7—C6—C5	119.5 (5)	C10—C11—H11	119.2

C3 ⁱⁱ —C3—N1	107.5 (3)	C9—C8—C7	121.9 (6)
C3 ⁱⁱ —C3—C2	122.2 (3)	C9—C8—H8	119
N1—C3—C2	130.2 (4)	C7—C8—H8	119
C1 ⁱⁱ —C1—C2	122.7 (3)	C10—C9—C8	119.1 (6)
C1 ⁱⁱ —C1—H1	118.7	C10—C9—H9	120.4
C2—C1—H1	118.7	C8—C9—H9	120.4
C1—C2—C3	115.1 (5)	C9—C10—C11	119.5 (6)
C1—C2—H2	122.5	C9—C10—H10	120.2
C3—C2—H2	122.5	C11—C10—H10	120.2
C3—N1—C4—N1 ⁱⁱ	0.1 (2)	C11—C6—C5—N1	123.0 (5)
C5—N1—C4—N1 ⁱⁱ	-177.2 (5)	C7—C6—C5—N1	-56.1 (7)
C4—N1—C3—C3 ⁱⁱ	-0.2 (6)	C11—C6—C7—C8	-1.0 (8)
C5—N1—C3—C3 ⁱⁱ	177.1 (5)	C5—C6—C7—C8	178.1 (5)
C4—N1—C3—C2	179.0 (4)	C7—C6—C11—C10	-0.5 (8)
C5—N1—C3—C2	-3.7 (8)	C5—C6—C11—C10	-179.6 (5)
C1 ⁱⁱ —C1—C2—C3	0.0 (9)	C6—C7—C8—C9	1.7 (10)
C3 ⁱⁱ —C3—C2—C1	-1.1 (8)	C7—C8—C9—C10	-0.8 (10)
N1—C3—C2—C1	179.8 (5)	C8—C9—C10—C11	-0.7 (10)
C4—N1—C5—C6	121.4 (5)	C6—C11—C10—C9	1.3 (9)
C3—N1—C5—C6	-55.4 (7)		

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