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catena-Poly[[chloridocadmium(II)]bis{μ-1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole}[chloridocadmium(II)]di-μ-chlorido]

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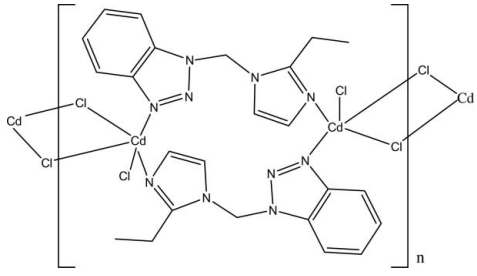
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.035; wR factor = 0.069; data-to-parameter ratio = 16.3.

In the polymeric title complex, $[CdCl_2(C_{12}H_{13}N_5)]_n$, the Cd^{II} atom is five-coordinated by two N atoms from two bridging 1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (bmei) ligands, two bridging Cl atoms and one terminal Cl atom in a distorted trigonal–bipyramidal geometry. The Cd^{II} atoms are connected alternately by the Cl atoms and bmei ligands, leading to a zigzag chain extending parallel to [011]. π–π interactions, with a centroid–centroid distance of 3.3016 (3) Å, help to stabilize the crystal packing.

Related literature

For similar compounds with symmetric or asymmetric *N*-heterocyclic ligands, see: Li *et al.* (2011); Hu *et al.* (2009); Meng *et al.* (2009); Huang *et al.* (2006).



Experimental

Crystal data

$[CdCl_2(C_{12}H_{13}N_5)]$
M_r = 410.57
Triclinic, $P\overline{1}$
a = 7.6055 (6) Å
b = 9.7027 (11) Å
c = 10.3144 (10) Å
α = 74.431 (9)°
β = 81.609 (7)°
γ = 87.720 (8)°
V = 725.36 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.87 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.993, T_{max} = 1.000
6082 measured reflections
2963 independent reflections
2534 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.069
S = 1.02
2963 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2490).

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supporting information

Acta Cryst. (2011). E**67**, m846 [doi:10.1107/S1600536811019908]

catena-Poly[[chloridocadmium(II)]bis{μ-1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole}[chloridocadmium(II)]di-μ-chlorido]

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S1. Comment

In coordination and supramolecular chemistry many symmetric imidazole and benzotriazole ligands have been applied (Li *et al.*, 2011; Hu *et al.*, 2009). However, studies involving asymmetric imidazole and benzotriazole ligands are rather rare (Meng *et al.*, 2009; Huang *et al.*, 2006). We were thus engaged in the synthesis of asymmetric N-heterocyclic ligands and synthesized the compound 1-[(1*H*-benzotriazol-1-yl)methyl]-1*H*-1,3-(2-ethyl-imidazol) (bmei). In this work, we selected this compound as a ligand for generation of the new complex $[Cd(C_{12}H_{13}N_5)Cl_2]_n$, (I), that is reported here.

In the complex (I) the Cd^{II} atom is five-coordinated by two N atoms from two bridging bmei ligands, two bridging Cl atoms and one terminal Cl atom in a distorted trigonal-bipyramidal geometry (Fig. 1). The two Cd^{II} ions are connected by a pair of bridging Cl atoms, yielding a centrosymmetric Cd_2Cl_2 binuclear unit with a Cd···Cd distance of 3.9657 (6) Å. The dimers are further linked by bmei ligands to give a zigzag chain extending parallel to [011] (Fig. 2). The distance between two Cd atoms bridged by the bmei ligand is 9.0727 (12) Å. In addition, the benzotriazole rings between adjacent chains are stacked in a face-to-face orientation with a centroid—centroid distance of 3.3016 (3) Å, so the crystal structure involves also π—π interactions.

S2. Experimental

The ligand 1-[(1*H*-benzotriazol-1-yl)methyl]-1*H*-1,3-(2-ethyl-imidazol) (0.04 mmol, 0.0096 g) in methanol (6 ml) was added dropwise to a methanol solution (5 ml) of $CdCl_2$ (0.04 mmol, 0.0074 g) in methanol. The resulting solution was allowed to stand at room temperature. After one week good quality colourless crystals were obtained and dried in air.

S3. Refinement

H atoms were placed geometrically and refined as riding atoms with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

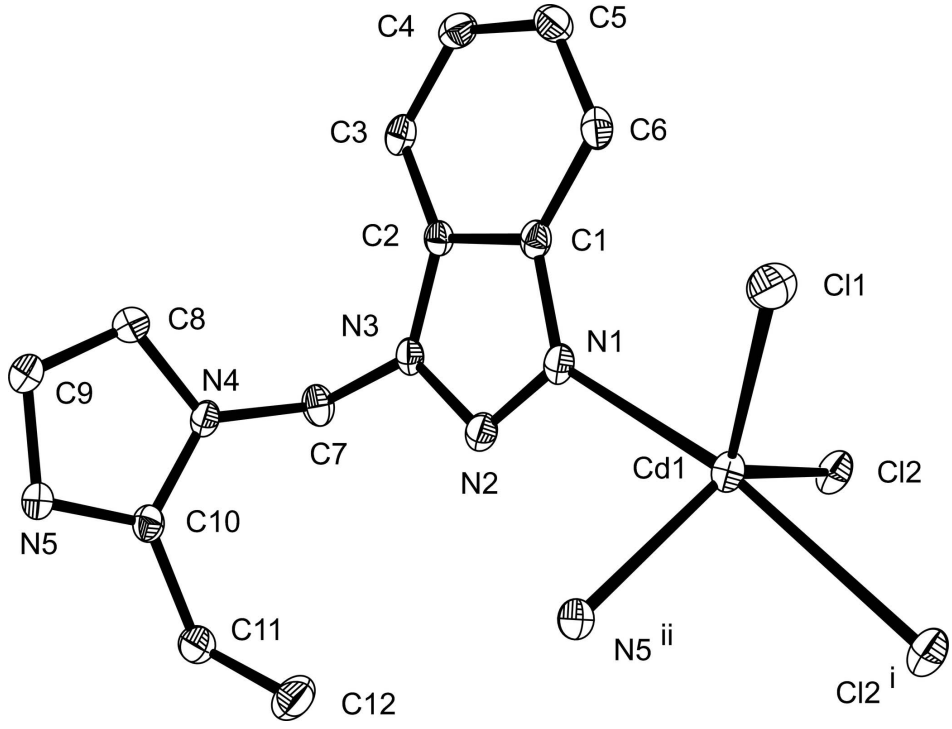

Figure 1

A fragment of the title complex, showing the coordination of the Cd^{II} atom with atom labelling of the non-H atoms and with 30% probability ellipsolids. [Symmetry codes: (i) -*x* + 1,-*y* + 1,-*z* + 1; (ii) -*x* + 1, -*y* + 2, -*z*.]

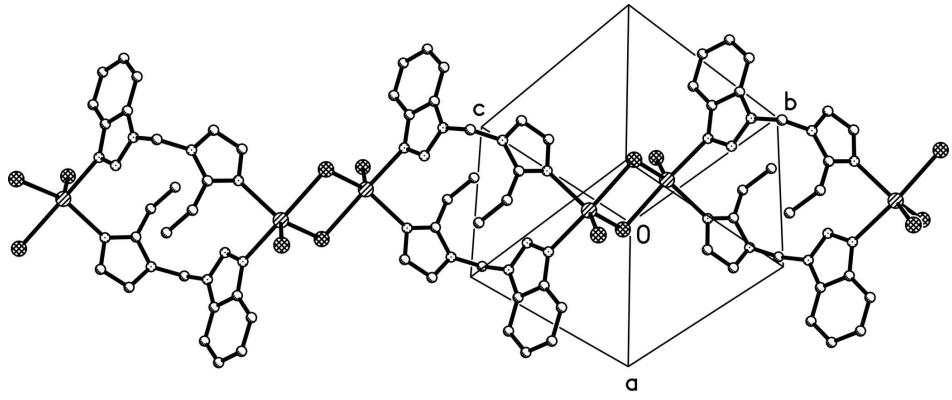

Figure 2

View of the zigzag chain structure of the title complex.

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β = 81.609 (7)°
γ = 87.720 (8)°
V = 725.36 (12) Å^3
Z = 2
F(000) = 404

D_x = 1.880 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.7107 Å
Cell parameters from 2806 reflections
θ = 3.2–26.3°
μ = 1.87 mm^{-1}
T = 293 K
Prismatic, colorless
0.20 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.993, T_{max} = 1.000
6082 measured reflections
2963 independent reflections
2534 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.3°, θ_{min} = 3.2°
h = −9→9
k = −12→11
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.069
S = 1.02
2963 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.37119 (4)	0.60250 (3)	0.34830 (3)	0.02594 (10)
Cl1	0.10727 (13)	0.49171 (10)	0.30891 (11)	0.0366 (3)
Cl2	0.41293 (13)	0.62093 (9)	0.58398 (10)	0.0321 (2)
N1	0.2477 (4)	0.8391 (3)	0.3168 (3)	0.0266 (7)
N2	0.3564 (4)	0.9476 (3)	0.2763 (3)	0.0270 (7)
N3	0.2578 (4)	1.0677 (3)	0.2711 (3)	0.0240 (7)
N4	0.3531 (4)	1.2614 (3)	0.0745 (3)	0.0268 (7)
N5	0.4535 (4)	1.3280 (3)	−0.1440 (3)	0.0302 (8)
C1	0.0746 (5)	0.8865 (4)	0.3398 (4)	0.0241 (8)
C2	0.0805 (5)	1.0354 (4)	0.3106 (4)	0.0223 (8)
C3	−0.0701 (5)	1.1177 (4)	0.3322 (4)	0.0267 (8)
H3	−0.0656	1.2167	0.3151	0.032*

C4	−0.2255 (5)	1.0418 (4)	0.3806 (4)	0.0303 (9)
H4	−0.3299	1.0915	0.3969	0.036*
C5	−0.2333 (5)	0.8923 (4)	0.4064 (4)	0.0322 (9)
H5	−0.3426	0.8466	0.4374	0.039*
C6	−0.0851 (5)	0.8122 (4)	0.3874 (4)	0.0281 (9)
H6	−0.0904	0.7132	0.4052	0.034*
C7	0.3445 (5)	1.2069 (4)	0.2205 (4)	0.0294 (9)
H7B	0.2797	1.2742	0.2643	0.035*
H7A	0.4640	1.1987	0.2442	0.035*
C8	0.2094 (5)	1.3085 (4)	0.0082 (4)	0.0345 (10)
H8	0.0919	1.3119	0.0479	0.041*
C9	0.2719 (5)	1.3492 (4)	−0.1261 (4)	0.0382 (10)
H9	0.2035	1.3856	−0.1954	0.046*
C10	0.4998 (5)	1.2744 (4)	−0.0210 (4)	0.0266 (8)
C11	0.6844 (5)	1.2391 (4)	0.0090 (4)	0.0365 (10)
H11B	0.7009	1.2715	0.0876	0.044*
H11A	0.7665	1.2922	−0.0674	0.044*
C12	0.7329 (6)	1.0793 (4)	0.0370 (4)	0.0457 (11)
H12A	0.7140	1.0451	−0.0389	0.069*
H12B	0.6593	1.0264	0.1173	0.069*
H12C	0.8555	1.0668	0.0502	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02975 (16)	0.02168 (16)	0.02519 (18)	0.00200 (11)	−0.00631 (12)	−0.00314 (12)
Cl1	0.0331 (5)	0.0287 (5)	0.0511 (7)	−0.0001 (4)	−0.0110 (5)	−0.0133 (5)
Cl2	0.0412 (6)	0.0275 (5)	0.0290 (6)	0.0108 (4)	−0.0100 (4)	−0.0087 (4)
N1	0.0333 (18)	0.0213 (16)	0.0227 (19)	0.0029 (14)	−0.0050 (14)	−0.0014 (13)
N2	0.0319 (18)	0.0236 (16)	0.0238 (19)	0.0048 (14)	−0.0044 (14)	−0.0038 (13)
N3	0.0314 (18)	0.0182 (15)	0.0197 (18)	0.0015 (13)	−0.0017 (14)	−0.0017 (13)
N4	0.0287 (17)	0.0235 (16)	0.0251 (19)	0.0018 (13)	−0.0074 (14)	0.0005 (13)
N5	0.0283 (18)	0.0332 (18)	0.0240 (19)	0.0025 (14)	−0.0036 (14)	0.0009 (14)
C1	0.031 (2)	0.0235 (19)	0.017 (2)	0.0042 (16)	−0.0018 (16)	−0.0045 (15)
C2	0.0267 (19)	0.0219 (19)	0.017 (2)	0.0004 (15)	−0.0028 (15)	−0.0036 (15)
C3	0.037 (2)	0.0228 (19)	0.021 (2)	0.0059 (17)	−0.0074 (17)	−0.0064 (16)
C4	0.027 (2)	0.036 (2)	0.028 (2)	0.0062 (17)	−0.0050 (17)	−0.0095 (18)
C5	0.029 (2)	0.036 (2)	0.029 (2)	−0.0055 (18)	−0.0010 (18)	−0.0051 (18)
C6	0.035 (2)	0.0225 (19)	0.025 (2)	−0.0036 (17)	−0.0068 (17)	−0.0011 (16)
C7	0.040 (2)	0.025 (2)	0.023 (2)	−0.0029 (17)	−0.0034 (18)	−0.0063 (17)
C8	0.027 (2)	0.036 (2)	0.035 (3)	0.0032 (18)	−0.0033 (18)	−0.0013 (19)
C9	0.030 (2)	0.045 (2)	0.032 (3)	0.0039 (19)	−0.0086 (19)	0.004 (2)
C10	0.030 (2)	0.0191 (18)	0.028 (2)	0.0003 (16)	−0.0031 (17)	−0.0019 (16)
C11	0.029 (2)	0.047 (3)	0.029 (2)	−0.0005 (19)	−0.0057 (18)	−0.002 (2)
C12	0.046 (3)	0.056 (3)	0.034 (3)	0.021 (2)	−0.012 (2)	−0.009 (2)

Geometric parameters (Å, º)

Cd1—Cl1	2.4482 (10)	C3—H3	0.9300
Cd1—Cl2^{i}	2.6687 (10)	C3—C4	1.374 (5)
Cd1—Cl2	2.5505 (10)	C4—H4	0.9300
Cd1—N1	2.403 (3)	C4—C5	1.405 (5)
Cd1—N5^{ii}	2.272 (3)	C5—H5	0.9300
Cl2—Cd1^{i}	2.6686 (10)	C5—C6	1.363 (5)
N1—N2	1.303 (4)	C6—H6	0.9300
N1—C1	1.386 (5)	C7—H7B	0.9700
N2—N3	1.353 (4)	C7—H7A	0.9700
N3—C2	1.374 (4)	C8—H8	0.9300
N3—C7	1.457 (4)	C8—C9	1.353 (5)
N4—C7	1.449 (5)	C9—H9	0.9300
N4—C8	1.371 (5)	C10—C11	1.488 (5)
N4—C10	1.362 (5)	C11—H11B	0.9700
N5—Cd1^{ii}	2.272 (3)	C11—H11A	0.9700
N5—C9	1.381 (5)	C11—C12	1.539 (5)
N5—C10	1.329 (5)	C12—H12A	0.9600
C1—C2	1.395 (5)	C12—H12B	0.9600
C1—C6	1.394 (5)	C12—H12C	0.9600
C2—C3	1.396 (5)		
Cd1—Cl2—Cd1^{i}	98.87 (3)	C3—C4—H4	118.6
Cl1—Cd1—Cl2^{i}	102.49 (3)	C3—C4—C5	122.8 (4)
Cl1—Cd1—Cl2	121.87 (4)	C4—C3—C2	115.1 (3)
Cl2—Cd1—Cl2^{i}	81.13 (3)	C4—C3—H3	122.5
N1—Cd1—Cl1	95.86 (8)	C4—C5—H5	119.1
N1—Cd1—Cl2	85.51 (8)	C5—C4—H4	118.6
N1—Cd1—Cl2^{i}	161.13 (8)	C5—C6—C1	116.5 (3)
N1—N2—N3	107.5 (3)	C5—C6—H6	121.7
N1—C1—C2	107.3 (3)	C6—C1—C2	121.3 (3)
N1—C1—C6	131.4 (3)	C6—C5—C4	121.8 (4)
N2—N1—Cd1	118.2 (2)	C6—C5—H5	119.1
N2—N1—C1	110.0 (3)	H7B—C7—H7A	107.9
N2—N3—C2	111.1 (3)	C8—N4—C7	124.7 (3)
N2—N3—C7	119.4 (3)	C8—C9—N5	109.1 (4)
N3—C2—C1	104.2 (3)	C8—C9—H9	125.4
N3—C2—C3	133.2 (3)	C9—N5—Cd1^{ii}	123.7 (3)
N3—C7—H7B	109.2	C9—C8—N4	106.6 (4)
N3—C7—H7A	109.2	C9—C8—H8	126.7
N4—C7—N3	112.0 (3)	C10—N4—C7	127.5 (3)
N4—C7—H7B	109.2	C10—N4—C8	107.9 (3)
N4—C7—H7A	109.2	C10—N5—Cd1^{ii}	129.2 (3)
N4—C8—H8	126.7	C10—N5—C9	106.8 (3)
N4—C10—C11	124.9 (4)	C10—C11—H11B	108.5
N5^{ii}—Cd1—Cl1	106.55 (8)	C10—C11—H11A	108.5
N5^{ii}—Cd1—Cl2^{i}	88.42 (8)	C10—C11—C12	115.0 (3)

N5^{ii}—Cd1—Cl2	131.58 (8)	C11—C12—H12A	109.5
N5^{ii}—Cd1—N1	90.57 (11)	C11—C12—H12B	109.5
N5—C9—H9	125.4	C11—C12—H12C	109.5
N5—C10—N4	109.5 (3)	H11B—C11—H11A	107.5
N5—C10—C11	125.5 (4)	C12—C11—H11B	108.5
C1—N1—Cd1	131.7 (2)	C12—C11—H11A	108.5
C1—C2—C3	122.5 (3)	H12A—C12—H12B	109.5
C1—C6—H6	121.7	H12A—C12—H12C	109.5
C2—N3—C7	129.5 (3)	H12B—C12—H12C	109.5
C2—C3—H3	122.5		

Cd1—N1—N2—N3	−177.7 (2)	N4—C10—C11—C12	81.6 (5)
Cd1—N1—C1—C2	176.9 (2)	N5^{ii}—Cd1—Cl2—Cd1^{i}	−79.87 (11)
Cd1—N1—C1—C6	−0.9 (6)	N5^{ii}—Cd1—N1—N2	−47.0 (3)
Cd1^{ii}—N5—C9—C8	−174.2 (2)	N5^{ii}—Cd1—N1—C1	136.3 (3)
Cd1^{ii}—N5—C10—N4	173.7 (2)	N5—C10—C11—C12	−100.9 (4)
Cd1^{ii}—N5—C10—C11	−4.0 (5)	C1—N1—N2—N3	−0.3 (4)
Cl1—Cd1—Cl2—Cd1^{i}	99.25 (4)	C1—C2—C3—C4	−1.8 (5)
Cl1—Cd1—N1—N2	−153.7 (2)	C2—N3—C7—N4	−87.5 (4)
Cl1—Cd1—N1—C1	29.6 (3)	C2—C1—C6—C5	−1.4 (5)
Cl2^{i}—Cd1—Cl2—Cd1^{i}	0.000 (2)	C2—C3—C4—C5	−0.1 (6)
Cl2^{i}—Cd1—N1—N2	39.8 (4)	C3—C4—C5—C6	1.3 (6)
Cl2—Cd1—N1—N2	84.7 (2)	C4—C5—C6—C1	−0.5 (6)
Cl2—Cd1—N1—C1	−92.0 (3)	C6—C1—C2—N3	178.3 (3)
Cl2^{i}—Cd1—N1—C1	−136.9 (3)	C6—C1—C2—C3	2.7 (6)
N1—Cd1—Cl2—Cd1^{i}	−166.64 (8)	C7—N3—C2—C1	175.8 (3)
N1—N2—N3—C2	0.5 (4)	C7—N3—C2—C3	−9.3 (6)
N1—N2—N3—C7	−176.2 (3)	C7—N4—C8—C9	−179.5 (3)
N1—C1—C2—N3	0.3 (4)	C7—N4—C10—N5	179.6 (3)
N1—C1—C2—C3	−175.3 (3)	C7—N4—C10—C11	−2.6 (6)
N1—C1—C6—C5	176.1 (4)	C8—N4—C7—N3	70.3 (4)
N2—N1—C1—C2	0.0 (4)	C8—N4—C10—N5	0.1 (4)
N2—N1—C1—C6	−177.7 (4)	C8—N4—C10—C11	177.9 (3)
N2—N3—C2—C1	−0.5 (4)	C9—N5—C10—N4	−0.2 (4)
N2—N3—C2—C3	174.4 (4)	C9—N5—C10—C11	−178.0 (3)
N2—N3—C7—N4	88.6 (4)	C10—N4—C7—N3	−109.1 (4)
N3—C2—C3—C4	−176.0 (4)	C10—N4—C8—C9	0.0 (4)
N4—C8—C9—N5	−0.1 (4)	C10—N5—C9—C8	0.2 (4)

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