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# *catena*-Poly[[dichloridoiron(II)]-$\mu$-4,4″-bis(benzimidazol-1-yl)-1,1′:4′,1″-terphenyl]

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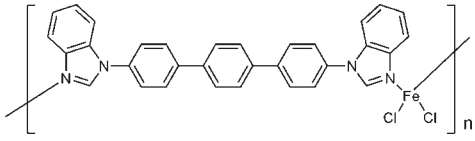
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.049; $wR$ factor = 0.117; data-to-parameter ratio = 12.5.

In the title coordination polymer, $[FeCl_2(C_{32}H_{22}N_4)]_n$, the $Fe^{II}$ atom lies on a crystallographic twofold axis and a distorted $FeCl_2N_2$ tetrahedral coordination geometry arises. The complete ligand is generated by crystallographic twofold symmetry, resulting in an infinite one-dimensional architecture along [101].

## Related literature

For background to benzimidazoles as ligands, see: Vijayan *et al.* (2006).




## Experimental

### Crystal data

$[FeCl_2(C_{32}H_{22}N_4)]$ $M_r$ = 589.29
Monoclinic, $C2/c$
$a$ = 14.519 (3) Å
$b$ = 14.303 (3) Å
$c$ = 12.461 (3) Å
$\beta$ = 101.94 (3)°
$V$ = 2531.6 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.84 mm$^{-1}$
$T$ = 293 K
0.20 × 0.18 × 0.15 mm

### Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.846, $T_{max}$ = 0.882
9515 measured reflections
2218 independent reflections
1960 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.052

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
$S$ = 1.12
2218 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Fe1—N1 | 2.076 (2) | Fe1—Cl1 | 2.2489 (10) |

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We thank the College Research Program of Yuncheng University [2008114] for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5310).

## References

Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vijayan, N., Bhagavannarayana, G., Balamurugan, N., Babu, R. R., Maurya, K. K., Gopalakrishnan, R. & Ramasamy, P. (2006). *J. Cryst. Growth*, **293**, 318–323.

# supporting information

*Acta Cryst.* (2010). E**66**, m267 [doi:10.1107/S1600536810002837]

## *catena*-Poly[[dichloridoiron(II)]-$\mu$-4,4′′-bis(benzimidazol-1-yl)-1,1′:4′,1′′-terphenyl]

**Hui Li, Zhuangwei Wei, Qiaojuan Gong and Qiuping Han**

### S1. Comment

Benzimidazole has been well used in crystal engineering, and a large number of benzimidazole-containing flexible ligands have been extensively studied. However, to our knowledge, the research on benzoimidazole ligands bearing rigid spacers is still less developed.

Single-crystal X-ray diffraction analysis reveals that the title compound crystallizes in the monoclinic space group *C*2/*c*. The geometry of the $Fe^{II}$ ion is surrounded by two benzimidazole rings of distinct **L** ligands and two chlorine anions, which illustrates a slightly distorted tetrahedral coordination environment (Fig. **1**). Notably, as shown in Fig. **2**, the four-coordinated $Fe^{II}$ center is bridged by the linear ligand **L** to form an infinite one-dimensional architecture along crystallographic [101] axis.

### S2. Experimental

A mixture of $(CH_3)_2CHOH$ and $CHCl_3$ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of 4,4′-Bis(benzimidazol-1-yl)terphenyl (**L**, 0.06 mmol) in $CHCl_3$ (6 ml). Then a solution of $FeCl_2$ (0.02 mmol) in $(CH_3)_2CHOH$ (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, yellow blocks of (I) appeared at the boundary. Yield: ~10% (based on **L**).

### S3. Refinement

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$.

The N-bound H atoms were located in a difference map and their positions were freely refined with $U_{iso}$(H) = 1.2$U_{eq}$(N).

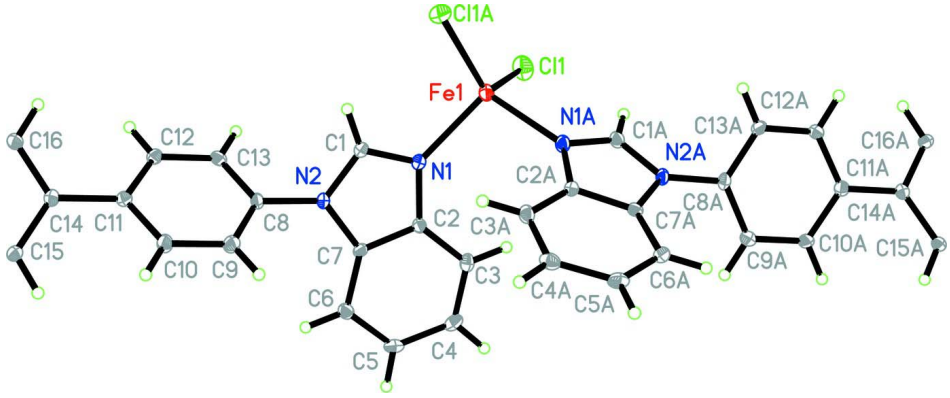



**Figure 1**

A fragment of a polymeric chain in (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

***catena*-Poly[[dichloridoiron(II)]-*μ*- 4,4′′-bis(benzimidazol-1-yl)-1,1′:4′,1′′-terphenyl]**

*Crystal data*

$[FeCl_2(C_{32}H_{22}N_4)]$
$M_r = 589.29$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 14.519\ (3)$ Å
$b = 14.303\ (3)$ Å
$c = 12.461\ (3)$ Å
$\beta = 101.94\ (3)°$
$V = 2531.6\ (9)$ Å$^3$
$Z = 4$
$F(000) = 1208$
$D_x = 1.546$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2574 reflections
$\theta = 2.0–27.9°$
$\mu = 0.84$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.20 × 0.18 × 0.15 mm

*Data collection*

Rigaku Saturn CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.846$, $T_{max} = 0.882$
9515 measured reflections
2218 independent reflections
1960 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -17\rightarrow16$
$k = -16\rightarrow15$
$l = -14\rightarrow14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.117$
$S = 1.12$
2218 reflections
177 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
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 2.1075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.41$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe1 | 0.0000 | 1.12084 (4) | 0.7500 | 0.0240 (2) |
| Cl1 | 0.02255 (6) | 1.20219 (6) | 0.90773 (8) | 0.0423 (3) |
| N2 | 0.20786 (16) | 0.96985 (16) | 0.63670 (19) | 0.0186 (6) |
| N1 | 0.10013 (17) | 1.02547 (17) | 0.72169 (19) | 0.0207 (6) |
| C15 | 0.4708 (2) | 0.8783 (2) | 0.2868 (2) | 0.0176 (6) |
| H15 | 0.4516 | 0.8216 | 0.3115 | 0.021* |
| C11 | 0.3788 (2) | 0.9625 (2) | 0.4047 (2) | 0.0181 (6) |
| C14 | 0.4398 (2) | 0.9609 (2) | 0.3250 (2) | 0.0185 (6) |
| C8 | 0.2661 (2) | 0.9662 (2) | 0.5587 (2) | 0.0187 (6) |
| C13 | 0.3223 (2) | 1.0412 (2) | 0.5485 (2) | 0.0183 (6) |
| H13 | 0.3231 | 1.0931 | 0.5937 | 0.022* |
| C3 | 0.1067 (2) | 0.8921 (2) | 0.8545 (2) | 0.0213 (7) |
| H3 | 0.0598 | 0.9141 | 0.8887 | 0.026* |
| C10 | 0.3213 (2) | 0.8878 (2) | 0.4174 (3) | 0.0228 (7) |
| H10 | 0.3212 | 0.8351 | 0.3736 | 0.027* |
| C1 | 0.1466 (2) | 1.0385 (2) | 0.6442 (2) | 0.0203 (7) |
| H1 | 0.1381 | 1.0905 | 0.5984 | 0.024* |
| C9 | 0.2649 (2) | 0.8892 (2) | 0.4924 (3) | 0.0233 (7) |
| H9 | 0.2261 | 0.8387 | 0.4986 | 0.028* |
| C16 | 0.4710 (2) | 1.0437 (2) | 0.2859 (2) | 0.0199 (6) |
| H16 | 0.4514 | 1.1005 | 0.3098 | 0.024* |
| C7 | 0.2006 (2) | 0.9061 (2) | 0.7177 (2) | 0.0171 (6) |
| C12 | 0.3767 (2) | 1.0395 (2) | 0.4721 (2) | 0.0184 (6) |
| H12 | 0.4137 | 1.0913 | 0.4647 | 0.022* |
| C2 | 0.1330 (2) | 0.9411 (2) | 0.7698 (2) | 0.0177 (6) |
| C5 | 0.2242 (2) | 0.7782 (2) | 0.8350 (2) | 0.0245 (7) |
| H5 | 0.2559 | 0.7235 | 0.8605 | 0.029* |
| C6 | 0.2490 (2) | 0.8247 (2) | 0.7494 (2) | 0.0212 (7) |
| H6 | 0.2957 | 0.8027 | 0.7149 | 0.025* |
| C4 | 0.1526 (2) | 0.8102 (2) | 0.8854 (2) | 0.0235 (7) |
| H4 | 0.1360 | 0.7750 | 0.9412 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0229 (4) | 0.0202 (4) | 0.0323 (4) | 0.000 | 0.0134 (3) | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl1 | 0.0413 (6) | 0.0368 (5) | 0.0522 (6) | −0.0083 (4) | 0.0174 (5) | −0.0199 (4) |
| N2 | 0.0184 (13) | 0.0194 (13) | 0.0205 (13) | 0.0010 (10) | 0.0099 (10) | 0.0014 (10) |
| N1 | 0.0213 (14) | 0.0203 (14) | 0.0226 (13) | 0.0014 (11) | 0.0097 (11) | 0.0035 (11) |
| C15 | 0.0176 (16) | 0.0168 (15) | 0.0187 (14) | −0.0018 (12) | 0.0041 (12) | 0.0017 (12) |
| C11 | 0.0186 (16) | 0.0178 (15) | 0.0182 (14) | 0.0007 (12) | 0.0043 (12) | 0.0020 (12) |
| C14 | 0.0170 (15) | 0.0204 (16) | 0.0185 (14) | −0.0008 (12) | 0.0047 (12) | 0.0003 (12) |
| C8 | 0.0172 (15) | 0.0216 (16) | 0.0192 (14) | 0.0036 (12) | 0.0082 (12) | 0.0026 (12) |
| C13 | 0.0190 (16) | 0.0155 (15) | 0.0203 (15) | 0.0014 (12) | 0.0041 (12) | −0.0030 (12) |
| C3 | 0.0202 (16) | 0.0266 (17) | 0.0182 (15) | −0.0030 (13) | 0.0066 (12) | −0.0023 (13) |
| C10 | 0.0272 (18) | 0.0191 (17) | 0.0253 (16) | −0.0050 (13) | 0.0125 (14) | −0.0069 (13) |
| C1 | 0.0193 (16) | 0.0190 (16) | 0.0242 (15) | 0.0009 (13) | 0.0081 (13) | 0.0044 (13) |
| C9 | 0.0243 (17) | 0.0193 (16) | 0.0281 (17) | −0.0046 (13) | 0.0097 (14) | −0.0021 (13) |
| C16 | 0.0224 (16) | 0.0167 (15) | 0.0218 (15) | −0.0004 (12) | 0.0074 (12) | −0.0023 (12) |
| C7 | 0.0199 (16) | 0.0134 (14) | 0.0189 (14) | −0.0024 (12) | 0.0057 (12) | 0.0013 (12) |
| C12 | 0.0183 (16) | 0.0171 (15) | 0.0200 (14) | −0.0018 (12) | 0.0044 (12) | 0.0004 (12) |
| C2 | 0.0159 (15) | 0.0170 (15) | 0.0211 (15) | 0.0003 (12) | 0.0058 (12) | −0.0011 (12) |
| C5 | 0.0288 (18) | 0.0147 (16) | 0.0284 (17) | 0.0007 (13) | 0.0018 (14) | 0.0025 (13) |
| C6 | 0.0203 (16) | 0.0185 (16) | 0.0257 (16) | 0.0001 (13) | 0.0066 (13) | −0.0037 (13) |
| C4 | 0.0315 (18) | 0.0207 (16) | 0.0181 (15) | −0.0060 (13) | 0.0048 (13) | 0.0024 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Fe1—N1$^{i}$ | 2.076 (2) | C13—H13 | 0.9300 |
| Fe1—N1 | 2.076 (2) | C3—C4 | 1.362 (4) |
| Fe1—Cl1$^{i}$ | 2.2489 (10) | C3—C2 | 1.384 (4) |
| Fe1—Cl1 | 2.2489 (10) | C3—H3 | 0.9300 |
| N2—C1 | 1.342 (4) | C10—C9 | 1.364 (4) |
| N2—C7 | 1.381 (4) | C10—H10 | 0.9300 |
| N2—C8 | 1.415 (4) | C1—H1 | 0.9300 |
| N1—C1 | 1.300 (4) | C9—H9 | 0.9300 |
| N1—C2 | 1.388 (4) | C16—C16$^{ii}$ | 1.349 (6) |
| C15—C15$^{ii}$ | 1.373 (6) | C16—H16 | 0.9300 |
| C15—C14 | 1.383 (4) | C7—C6 | 1.375 (4) |
| C15—H15 | 0.9300 | C7—C2 | 1.379 (4) |
| C11—C10 | 1.386 (4) | C12—H12 | 0.9300 |
| C11—C12 | 1.389 (4) | C5—C6 | 1.367 (4) |
| C11—C14 | 1.461 (4) | C5—C4 | 1.398 (4) |
| C14—C16 | 1.392 (4) | C5—H5 | 0.9300 |
| C8—C13 | 1.368 (4) | C6—H6 | 0.9300 |
| C8—C9 | 1.375 (4) | C4—H4 | 0.9300 |
| C13—C12 | 1.358 (4) | | |
| | | | |
| N1$^{i}$—Fe1—N1 | 97.86 (13) | C9—C10—C11 | 121.9 (3) |
| N1$^{i}$—Fe1—Cl1$^{i}$ | 120.53 (7) | C9—C10—H10 | 119.1 |
| N1—Fe1—Cl1$^{i}$ | 99.90 (7) | C11—C10—H10 | 119.1 |
| N1$^{i}$—Fe1—Cl1 | 99.90 (7) | N1—C1—N2 | 113.6 (3) |
| N1—Fe1—Cl1 | 120.53 (7) | N1—C1—H1 | 123.2 |
| Cl1$^{i}$—Fe1—Cl1 | 117.69 (6) | N2—C1—H1 | 123.2 |

| | | | |
|---|---|---|---|
| C1—N2—C7 | 106.3 (2) | C10—C9—C8 | 119.3 (3) |
| C1—N2—C8 | 125.0 (2) | C10—C9—H9 | 120.4 |
| C7—N2—C8 | 128.6 (2) | C8—C9—H9 | 120.4 |
| C1—N1—C2 | 105.1 (2) | C16$^{ii}$—C16—C14 | 121.72 (17) |
| C1—N1—Fe1 | 121.4 (2) | C16$^{ii}$—C16—H16 | 119.1 |
| C2—N1—Fe1 | 133.50 (19) | C14—C16—H16 | 119.1 |
| C15$^{ii}$—C15—C14 | 121.33 (17) | C6—C7—C2 | 122.9 (3) |
| C15$^{ii}$—C15—H15 | 119.3 | C6—C7—N2 | 131.2 (3) |
| C14—C15—H15 | 119.3 | C2—C7—N2 | 105.9 (2) |
| C10—C11—C12 | 117.0 (3) | C13—C12—C11 | 121.8 (3) |
| C10—C11—C14 | 122.0 (3) | C13—C12—H12 | 119.1 |
| C12—C11—C14 | 121.0 (3) | C11—C12—H12 | 119.1 |
| C15—C14—C16 | 117.0 (3) | C7—C2—C3 | 120.7 (3) |
| C15—C14—C11 | 122.2 (3) | C7—C2—N1 | 109.1 (2) |
| C16—C14—C11 | 120.8 (3) | C3—C2—N1 | 130.2 (3) |
| C13—C8—C9 | 120.3 (3) | C6—C5—C4 | 122.1 (3) |
| C13—C8—N2 | 119.2 (3) | C6—C5—H5 | 118.9 |
| C9—C8—N2 | 120.5 (3) | C4—C5—H5 | 118.9 |
| C12—C13—C8 | 119.7 (3) | C5—C6—C7 | 115.8 (3) |
| C12—C13—H13 | 120.1 | C5—C6—H6 | 122.1 |
| C8—C13—H13 | 120.1 | C7—C6—H6 | 122.1 |
| C4—C3—C2 | 117.1 (3) | C3—C4—C5 | 121.3 (3) |
| C4—C3—H3 | 121.5 | C3—C4—H4 | 119.3 |
| C2—C3—H3 | 121.5 | C5—C4—H4 | 119.3 |

| | | | |
|---|---|---|---|
| N1$^{i}$—Fe1—N1—C1 | 139.0 (3) | N2—C8—C9—C10 | 179.6 (3) |
| Cl1$^{i}$—Fe1—N1—C1 | 16.0 (2) | C15—C14—C16—C16$^{ii}$ | −0.1 (5) |
| Cl1—Fe1—N1—C1 | −114.6 (2) | C11—C14—C16—C16$^{ii}$ | 178.6 (3) |
| N1$^{i}$—Fe1—N1—C2 | −40.2 (2) | C1—N2—C7—C6 | −177.4 (3) |
| Cl1$^{i}$—Fe1—N1—C2 | −163.2 (3) | C8—N2—C7—C6 | 3.3 (5) |
| Cl1—Fe1—N1—C2 | 66.2 (3) | C1—N2—C7—C2 | 0.4 (3) |
| C15$^{ii}$—C15—C14—C16 | −0.3 (5) | C8—N2—C7—C2 | −178.9 (3) |
| C15$^{ii}$—C15—C14—C11 | −179.0 (3) | C8—C13—C12—C11 | −1.3 (4) |
| C10—C11—C14—C15 | −23.9 (4) | C10—C11—C12—C13 | 1.1 (4) |
| C12—C11—C14—C15 | 155.5 (3) | C14—C11—C12—C13 | −178.3 (3) |
| C10—C11—C14—C16 | 157.5 (3) | C6—C7—C2—C3 | −3.6 (5) |
| C12—C11—C14—C16 | −23.2 (4) | N2—C7—C2—C3 | 178.3 (3) |
| C1—N2—C8—C13 | 53.0 (4) | C6—C7—C2—N1 | 177.6 (3) |
| C7—N2—C8—C13 | −127.8 (3) | N2—C7—C2—N1 | −0.5 (3) |
| C1—N2—C8—C9 | −125.7 (3) | C4—C3—C2—C7 | 2.0 (4) |
| C7—N2—C8—C9 | 53.5 (4) | C4—C3—C2—N1 | −179.4 (3) |
| C9—C8—C13—C12 | 0.3 (4) | C1—N1—C2—C7 | 0.4 (3) |
| N2—C8—C13—C12 | −178.4 (3) | Fe1—N1—C2—C7 | 179.6 (2) |
| C12—C11—C10—C9 | 0.1 (5) | C1—N1—C2—C3 | −178.3 (3) |
| C14—C11—C10—C9 | 179.5 (3) | Fe1—N1—C2—C3 | 1.0 (5) |
| C2—N1—C1—N2 | −0.1 (3) | C4—C5—C6—C7 | 1.4 (4) |
| Fe1—N1—C1—N2 | −179.48 (19) | C2—C7—C6—C5 | 1.8 (4) |
| C7—N2—C1—N1 | −0.2 (3) | N2—C7—C6—C5 | 179.3 (3) |

| | | | |
|---|---|---|---|
| C8—N2—C1—N1 | 179.1 (3) | C2—C3—C4—C5 | 1.1 (4) |
| C11—C10—C9—C8 | −1.2 (5) | C6—C5—C4—C3 | −2.9 (5) |
| C13—C8—C9—C10 | 0.9 (5) | | |

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