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# 1,4-Dihexyloxy-2,5-bis(2-nitrophenyl)benzene

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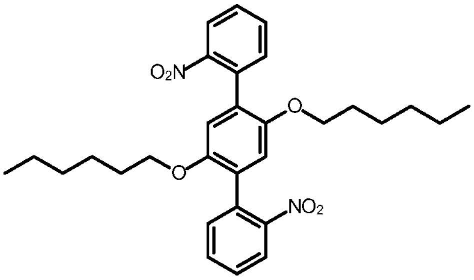
Key indicators: single-crystal X-ray study; $T$ = 193 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.044; $wR$ factor = 0.120; data-to-parameter ratio = 19.3.

The title compound, $C_{30}H_{36}N_2O_6$, was prepared *via* twofold Suzuki coupling of a diboronic acid with bromonitrobenzene. The molecule is located on a crystallographic inversion centre. The lateral benzene ring and the central ring make a dihedral angle of 48.75 (14)° and the nitro group is twisted by 41.47 (13)° out of the plane of the benzene ring. The nitro and hexyloxy groups are in close proximity and the hexyloxy chain adopts an all-*anti* conformation.

## Related literature

For the synthesis of carbazoles and heteroanalogous carbazoles, see: Letessier *et al.* (2011); Dassonneville *et al.* (2011); Nissen & Detert (2011); Letessier & Detert (2012). For the Cadogan reaction, see: Cadogan (1962). For Suzuki cross-couplings see Miyaura & Suzuki (1995). For $\pi$-systems for optoelectronic applications, see: Nemkovich *et al.* (2009). For structures of substituted $p$-terphenyls, see: Jones *et al.* (2005), Moschel *et al.* (2011). For torsion in biphenyls, see: Miao *et al.* (2009); Fischer *et al.* (2007).



## Experimental

### Crystal data

$C_{30}H_{36}N_2O_6$
$M_r$ = 520.61
Monoclinic, $P2_1/n$
$a$ = 7.9314 (4) Å
$b$ = 19.2029 (17) Å
$c$ = 9.1247 (5) Å
$\beta$ = 96.368 (5)°
$V$ = 1381.17 (16) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 193 K
0.44 × 0.30 × 0.20 mm

### Data collection

Stoe IPDS 2T diffractometer
8154 measured reflections
3331 independent reflections
2610 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
$S$ = 1.07
3331 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.27 e Å$^{-3}$

Data collection: *X-AREA* (Stoe & Cie, 2011); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2011); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

The authors are grateful to Heinz Kolshorn for invaluable discussions and the NMR spectra.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5839).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1022 [doi:10.1107/S1600536812009944]

## 1,4-Dihexyloxy-2,5-bis(2-nitrophenyl)benzene

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### Comment

As part of a larger project on the synthesis of carbazoles and heteroanalogous carbazoles (Letessier *et al.* 2011, Dassonneville *et al.* 2011, Nissen & Detert 2011, Letessier & Detert 2012) the Cadogan reaction (Cadogan 1962) appeared to be a suitable method for the construction of larger planar $\pi$-systems for optoelectronic applications (Nemkovich *et al.* 2009). The title compond was prepared as an intermediate for the synthesis of dihexyloxy-indolocarbazole.

The title compound crystallizes in a centrosymmetrical conformation with a highly twisted dinitroterphenyl core and hexyloxy chains in an *all-anti* conformation. The dihedral angle of the mean planes of the central and the lateral ring is 131.25 (14)° with the *ortho*-substituents nitro- and hexyloxy in close proximity. The distance N10 - O13 (nitro-hexyloxy) is only 2.710 (2) Å. The nitro group is twisted out of the plane of the adjacent benzene ring, the dihedral angle is 138.53 (13)° pointing towards the adjacent *o*-hexyloxy group. A *o*-methyl substitution on on a biphenyl linkage is sufficient to open the dihedral angle from 9.45 ° (Fischer *et al.* 2007) to more than 63° (Jones *et al.* 2005). The twist (131.25°) found in the title compound - though *o*,*o*-disubstituted on both biphenyl linkages - is significantly smaller. This can result from an electronic attraction between N10 (nitro) and O13 (hexyloxy). Miao *et al.* (2009) reported a dihedral angle of 60.5° in the fourfold *o*-substituted 2,2-dimethoxy-6,6-dinitrobiphenyl.

### Experimental

Synthesis: A mixture of 2,5-dihexyloxy-1,4-phenylenediboronic acid (500 mg, 1.37 mmol), 1-bromo-2-nitrobenzene (553 mg, 2.74 mmol), $Pd(PPh_3)_3$ (79 mg, 0.067 mmol) in dimethoxyethane (10 ml) was stirred for 45 min at 298 K. An aqueous solution of $Na_2CO_3$ (1*M*, 8.2 ml) was added and the mixture heated to 353 K for 18 h. The cooled mixture was poured into water (40 ml) and the product was isolated by extraction with dichloromethane (3 *x* 15 ml), washing the pooled solutions with brine (2 *x* 10 ml), drying ($Na_2SO_4$) and crystallization from chloroform/pentane. Yield: 495 mg (70%) of a yellow solid with m. p. 438 - 440 K. $R_f = 0.41$ (silica gel, petroleum ether/ethyl acetate 9/1).

### Refinement

Hydrogen atoms were placed at calculated positions with C—H = 0.95 Å (aromatic) or 0.98–0.99 Å ($sp^3$ C-atom). All H atoms were refined in the riding-model approximation with isotropic displacement parameters set at 1.2–1.5 times of the $U_{eq}$ of the parent atom.

### Computing details

Data collection: *X-AREA* (Stoe & Cie, 2011); cell refinement: *X-AREA* (Stoe & Cie, 2011); data reduction: *X-RED* (Stoe & Cie, 2011); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

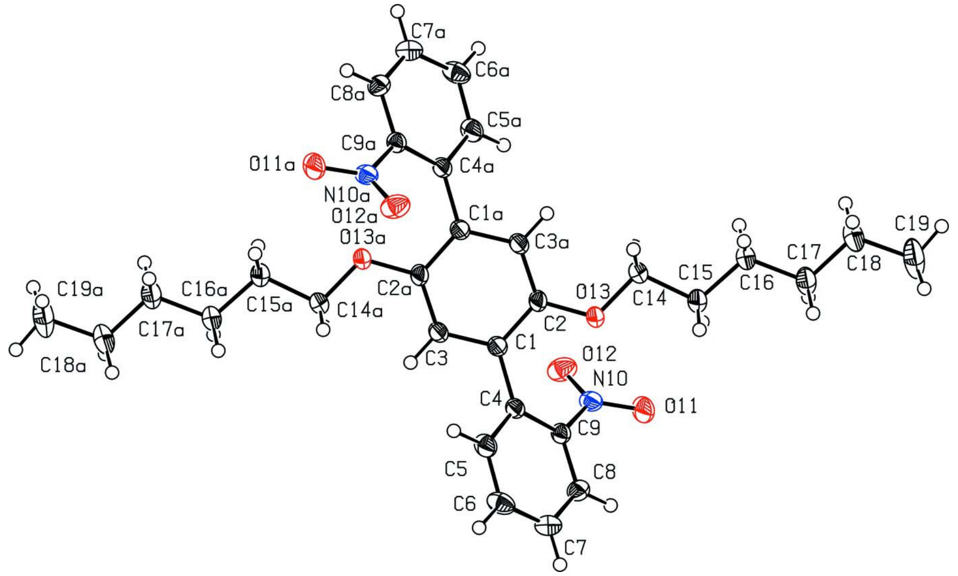

**Figure 1**

View of compound **I**. Displacement ellipsoids are drawn at the 50% probability level. Second part of the molecule labeled with *a* generated applying symmetry code 1 - *x*, 1 - *y*, 1 - *z*.

## 1,4-Dihexyloxy-2,5-bis(2-nitrophenyl)benzene

### *Crystal data*

$C_{30}H_{36}N_2O_6$
$M_r = 520.61$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9314\ (4)$ Å
$b = 19.2029\ (17)$ Å
$c = 9.1247\ (5)$ Å
$\beta = 96.368\ (5)°$
$V = 1381.17\ (16)$ Å$^3$
$Z = 2$
$F(000) = 556$
$D_x = 1.252$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7928 reflections
$\theta = 3.2–29.1°$
$\mu = 0.09$ mm$^{-1}$
$T = 193$ K
Block, yellow
0.44 × 0.30 × 0.20 mm

### *Data collection*

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm$^{-1}$
$\omega$ scan
8154 measured reflections
3331 independent reflections
2610 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.026$
$\theta_{\text{max}} = 28.0°$, $\theta_{\text{min}} = 3.2°$
$h = -10 \rightarrow 10$
$k = -25 \rightarrow 22$
$l = -12 \rightarrow 10$

### *Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.120$
$S = 1.07$
3331 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.4038P]$
  where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.27$ e Å$^{-3}$

*Special details*

**Experimental**. $^1$H-NMR (400 MHz, CDCl$_3$): $\delta$ = 7.95 (dd, $^3$J = 8.5 Hz, $^4$J= 1.2 Hz, 2 H, 3-H); 7.64 (dt, $^3$J = 7.5 Hz, $^4$J = 1.4 Hz, 2 H, 4-H); 7.49 - 7.45 (m, 4 H); 6.83 (s, 2 H, 2-H); 3.81 (bs (*t*), 4 H, O—CH$_2$); 1.59 - 1.54 (m, 4 H); 1.25 - 1.18 (m, 12 H); 0.80 (t, $^3$J = 6.9 Hz, 6 H, CH$_3$).
$^{13}$C-NMR (75 MHz, CDCl$_3$): $\delta$ = 149.7 (s, 2-C), 149.5 (*s*), 132.9 (*s*), 132.6 (*d*), 132.5 (*d*), 128.1 (*d*), 127.8 (*s*), 123.9 (*d*), 113.4 (*d*), 69.1 (*t*), 31.3 (*t*), 28.8 (*t*), 25.4 (*t*), 22.5 (*t*), 13.8 (*q*).
IR (ATR): $v$ = 3734, 3585, 3070, 2944, 2869, 2855, 2363, 2334, 1608, 1573, 1530, 1510, 1469, 1441, 1387, 1358, 1290, 1255, 1209, 1165, 1144, 1025, 997, 870, 860.
MS (EI): m/*z* = 520 (100%, $M^{+\cdot}$).

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.46215 (15) | 0.52525 (7) | 0.35512 (14) | 0.0240 (3) |
| C2 | 0.35820 (15) | 0.54228 (7) | 0.46442 (14) | 0.0252 (3) |
| C3 | 0.60362 (16) | 0.48321 (8) | 0.39358 (14) | 0.0264 (3) |
| H3 | 0.6756 | 0.4717 | 0.3206 | 0.032* |
| C4 | 0.43305 (15) | 0.55452 (7) | 0.20336 (14) | 0.0232 (3) |
| C5 | 0.57076 (16) | 0.58310 (8) | 0.14150 (15) | 0.0299 (3) |
| H5 | 0.6801 | 0.5811 | 0.1956 | 0.036* |
| C6 | 0.55321 (18) | 0.61424 (8) | 0.00394 (16) | 0.0338 (3) |
| H6 | 0.6502 | 0.6318 | −0.0362 | 0.041* |
| C7 | 0.39481 (18) | 0.61991 (8) | −0.07522 (16) | 0.0309 (3) |
| H7 | 0.3820 | 0.6432 | −0.1676 | 0.037* |
| C8 | 0.25493 (17) | 0.59149 (7) | −0.01925 (15) | 0.0273 (3) |
| H8 | 0.1456 | 0.5945 | −0.0732 | 0.033* |
| C9 | 0.27660 (15) | 0.55862 (7) | 0.11640 (14) | 0.0225 (3) |
| N10 | 0.12608 (13) | 0.52343 (6) | 0.16019 (12) | 0.0271 (3) |
| O11 | −0.01207 (12) | 0.55180 (6) | 0.13048 (12) | 0.0381 (3) |
| O12 | 0.14470 (14) | 0.46637 (6) | 0.21901 (12) | 0.0380 (3) |
| O13 | 0.22425 (12) | 0.58564 (6) | 0.42244 (10) | 0.0314 (2) |
| C14 | 0.11269 (18) | 0.60345 (9) | 0.52871 (16) | 0.0330 (3) |
| H14A | 0.1748 | 0.6300 | 0.6106 | 0.040* |
| H14B | 0.0665 | 0.5607 | 0.5699 | 0.040* |
| C15 | −0.02962 (17) | 0.64694 (9) | 0.45359 (16) | 0.0330 (3) |
| H15A | 0.0189 | 0.6874 | 0.4055 | 0.040* |
| H15B | −0.0946 | 0.6188 | 0.3758 | 0.040* |
| C16 | −0.1481 (2) | 0.67270 (12) | 0.5597 (2) | 0.0560 (6) |
| H16A | −0.1793 | 0.6328 | 0.6201 | 0.067* |

| | | | | |
|---|---|---|---|---|
| H16B | −0.0862 | 0.7067 | 0.6274 | 0.067* |
| C17 | −0.30865 (18) | 0.70652 (8) | 0.49024 (18) | 0.0344 (3) |
| H17A | −0.2781 | 0.7465 | 0.4299 | 0.041* |
| H17B | −0.3715 | 0.6726 | 0.4231 | 0.041* |
| C18 | −0.4239 (3) | 0.73189 (14) | 0.5993 (3) | 0.0670 (7) |
| H18A | −0.4492 | 0.6924 | 0.6631 | 0.080* |
| H18B | −0.3626 | 0.7675 | 0.6632 | 0.080* |
| C19 | −0.5889 (2) | 0.76264 (11) | 0.5319 (3) | 0.0602 (6) |
| H19A | −0.5662 | 0.8048 | 0.4767 | 0.090* |
| H19B | −0.6592 | 0.7745 | 0.6101 | 0.090* |
| H19C | −0.6488 | 0.7287 | 0.4650 | 0.090* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0190 (5) | 0.0341 (7) | 0.0187 (6) | 0.0020 (5) | 0.0005 (4) | −0.0030 (5) |
| C2 | 0.0172 (5) | 0.0358 (7) | 0.0218 (6) | 0.0056 (5) | −0.0005 (4) | −0.0031 (5) |
| C3 | 0.0204 (6) | 0.0391 (7) | 0.0199 (6) | 0.0049 (5) | 0.0027 (5) | −0.0037 (5) |
| C4 | 0.0202 (5) | 0.0296 (6) | 0.0198 (6) | 0.0027 (5) | 0.0023 (4) | −0.0032 (5) |
| C5 | 0.0189 (6) | 0.0436 (8) | 0.0271 (7) | −0.0031 (5) | 0.0017 (5) | −0.0039 (6) |
| C6 | 0.0302 (7) | 0.0441 (8) | 0.0285 (7) | −0.0111 (6) | 0.0094 (6) | −0.0021 (6) |
| C7 | 0.0375 (7) | 0.0326 (7) | 0.0229 (6) | −0.0045 (6) | 0.0040 (5) | 0.0024 (5) |
| C8 | 0.0260 (6) | 0.0322 (7) | 0.0228 (6) | 0.0003 (5) | −0.0010 (5) | 0.0010 (5) |
| C9 | 0.0186 (5) | 0.0268 (6) | 0.0219 (6) | −0.0002 (5) | 0.0020 (4) | −0.0012 (5) |
| N10 | 0.0210 (5) | 0.0398 (7) | 0.0201 (5) | −0.0036 (5) | 0.0009 (4) | −0.0006 (5) |
| O11 | 0.0178 (4) | 0.0605 (7) | 0.0353 (6) | 0.0027 (4) | 0.0006 (4) | −0.0021 (5) |
| O12 | 0.0358 (5) | 0.0425 (6) | 0.0351 (6) | −0.0098 (5) | 0.0014 (4) | 0.0114 (5) |
| O13 | 0.0239 (4) | 0.0492 (6) | 0.0213 (5) | 0.0155 (4) | 0.0029 (4) | 0.0003 (4) |
| C14 | 0.0277 (6) | 0.0471 (9) | 0.0254 (7) | 0.0141 (6) | 0.0078 (5) | 0.0025 (6) |
| C15 | 0.0248 (6) | 0.0453 (8) | 0.0288 (7) | 0.0118 (6) | 0.0030 (5) | 0.0009 (6) |
| C16 | 0.0502 (10) | 0.0811 (14) | 0.0402 (9) | 0.0427 (10) | 0.0203 (8) | 0.0197 (9) |
| C17 | 0.0254 (6) | 0.0330 (7) | 0.0459 (9) | 0.0059 (6) | 0.0090 (6) | 0.0019 (6) |
| C18 | 0.0543 (11) | 0.0902 (16) | 0.0615 (13) | 0.0435 (11) | 0.0297 (10) | 0.0211 (12) |
| C19 | 0.0324 (8) | 0.0556 (12) | 0.0951 (17) | 0.0150 (8) | 0.0188 (10) | 0.0009 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C3 | 1.3952 (18) | O13—C14 | 1.4250 (15) |
| C1—C2 | 1.4014 (17) | C14—C15 | 1.5065 (19) |
| C1—C4 | 1.4886 (18) | C14—H14A | 0.9900 |
| C2—O13 | 1.3705 (15) | C14—H14B | 0.9900 |
| C2—C3$^{i}$ | 1.3867 (19) | C15—C16 | 1.506 (2) |
| C3—C2$^{i}$ | 1.3867 (19) | C15—H15A | 0.9900 |
| C3—H3 | 0.9500 | C15—H15B | 0.9900 |
| C4—C5 | 1.3963 (18) | C16—C17 | 1.505 (2) |
| C4—C9 | 1.3990 (17) | C16—H16A | 0.9900 |
| C5—C6 | 1.383 (2) | C16—H16B | 0.9900 |
| C5—H5 | 0.9500 | C17—C18 | 1.505 (2) |
| C6—C7 | 1.382 (2) | C17—H17A | 0.9900 |
| C6—H6 | 0.9500 | C17—H17B | 0.9900 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.3838 (19) | C18—C19 | 1.503 (3) |
| C7—H7 | 0.9500 | C18—H18A | 0.9900 |
| C8—C9 | 1.3831 (18) | C18—H18B | 0.9900 |
| C8—H8 | 0.9500 | C19—H19A | 0.9800 |
| C9—N10 | 1.4655 (16) | C19—H19B | 0.9800 |
| N10—O12 | 1.2218 (16) | C19—H19C | 0.9800 |
| N10—O11 | 1.2268 (15) | | |

| | | | |
|---|---|---|---|
| C3—C1—C2 | 118.44 (12) | O13—C14—H14B | 110.0 |
| C3—C1—C4 | 119.33 (11) | C15—C14—H14B | 110.0 |
| C2—C1—C4 | 122.08 (11) | H14A—C14—H14B | 108.4 |
| O13—C2—C3$^{i}$ | 123.90 (11) | C16—C15—C14 | 112.27 (12) |
| O13—C2—C1 | 116.22 (11) | C16—C15—H15A | 109.2 |
| C3$^{i}$—C2—C1 | 119.85 (12) | C14—C15—H15A | 109.2 |
| C2$^{i}$—C3—C1 | 121.70 (11) | C16—C15—H15B | 109.2 |
| C2$^{i}$—C3—H3 | 119.2 | C14—C15—H15B | 109.2 |
| C1—C3—H3 | 119.2 | H15A—C15—H15B | 107.9 |
| C5—C4—C9 | 115.65 (12) | C17—C16—C15 | 115.45 (14) |
| C5—C4—C1 | 118.49 (11) | C17—C16—H16A | 108.4 |
| C9—C4—C1 | 125.82 (11) | C15—C16—H16A | 108.4 |
| C6—C5—C4 | 122.16 (12) | C17—C16—H16B | 108.4 |
| C6—C5—H5 | 118.9 | C15—C16—H16B | 108.4 |
| C4—C5—H5 | 118.9 | H16A—C16—H16B | 107.5 |
| C7—C6—C5 | 120.15 (12) | C18—C17—C16 | 114.11 (15) |
| C7—C6—H6 | 119.9 | C18—C17—H17A | 108.7 |
| C5—C6—H6 | 119.9 | C16—C17—H17A | 108.7 |
| C6—C7—C8 | 119.71 (13) | C18—C17—H17B | 108.7 |
| C6—C7—H7 | 120.1 | C16—C17—H17B | 108.7 |
| C8—C7—H7 | 120.1 | H17A—C17—H17B | 107.6 |
| C9—C8—C7 | 119.02 (12) | C19—C18—C17 | 114.93 (19) |
| C9—C8—H8 | 120.5 | C19—C18—H18A | 108.5 |
| C7—C8—H8 | 120.5 | C17—C18—H18A | 108.5 |
| C8—C9—C4 | 123.21 (12) | C19—C18—H18B | 108.5 |
| C8—C9—N10 | 115.49 (11) | C17—C18—H18B | 108.5 |
| C4—C9—N10 | 121.17 (11) | H18A—C18—H18B | 107.5 |
| O12—N10—O11 | 123.84 (12) | C18—C19—H19A | 109.5 |
| O12—N10—C9 | 118.09 (11) | C18—C19—H19B | 109.5 |
| O11—N10—C9 | 118.01 (12) | H19A—C19—H19B | 109.5 |
| C2—O13—C14 | 118.44 (10) | C18—C19—H19C | 109.5 |
| O13—C14—C15 | 108.30 (11) | H19A—C19—H19C | 109.5 |
| O13—C14—H14A | 110.0 | H19B—C19—H19C | 109.5 |
| C15—C14—H14A | 110.0 | | |

| | | | |
|---|---|---|---|
| C3—C1—C2—O13 | 177.82 (12) | C7—C8—C9—N10 | −173.60 (12) |
| C4—C1—C2—O13 | 2.17 (19) | C5—C4—C9—C8 | −3.0 (2) |
| C3—C1—C2—C3$^{i}$ | −0.7 (2) | C1—C4—C9—C8 | 174.57 (13) |
| C4—C1—C2—C3$^{i}$ | −176.30 (13) | C5—C4—C9—N10 | 172.61 (12) |
| C2—C1—C3—C2$^{i}$ | 0.7 (2) | C1—C4—C9—N10 | −9.8 (2) |
| C4—C1—C3—C2$^{i}$ | 176.44 (13) | C8—C9—N10—O12 | 138.53 (13) |

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|---|---|---|---|
| C3—C1—C4—C5 | −44.37 (18) | C4—C9—N10—O12 | −37.39 (18) |
| C2—C1—C4—C5 | 131.25 (14) | C8—C9—N10—O11 | −38.71 (17) |
| C3—C1—C4—C9 | 138.15 (14) | C4—C9—N10—O11 | 145.37 (13) |
| C2—C1—C4—C9 | −46.2 (2) | C3$^{i}$—C2—O13—C14 | −2.8 (2) |
| C9—C4—C5—C6 | 0.8 (2) | C1—C2—O13—C14 | 178.78 (13) |
| C1—C4—C5—C6 | −176.95 (13) | C2—O13—C14—C15 | −176.02 (12) |
| C4—C5—C6—C7 | 2.1 (2) | O13—C14—C15—C16 | −175.95 (16) |
| C5—C6—C7—C8 | −2.9 (2) | C14—C15—C16—C17 | −170.43 (16) |
| C6—C7—C8—C9 | 0.8 (2) | C15—C16—C17—C18 | −179.81 (19) |
| C7—C8—C9—C4 | 2.2 (2) | C16—C17—C18—C19 | −177.1 (2) |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.