organic compounds

A new crystal phase of $N,N,N′,N′$-tetraphenyl-1,1′-biphenyl-4,4′-diamine

Xiangfeng Shao,[a] Kenshiro Asahi,[a] Takayoshi Yamauchi,[a] Toyonari Sugimoto[a]* and Motoo Shiro[b]

[a]Department of Chemistry, Graduate School of Science, Osaka Prefecture University, Sakai, Osaka 599-8570, Japan, and [b]Rigaku Co., Akishima, Tokyo 196-8666, Japan
Correspondence e-mail: toyonari@c.s.osakafu-u.ac.jp

The complete molecule of the title compound, $C_{36}H_{28}N_2$, is generated by a crystallographic centre of inversion. The biphenyl unit is forced by symmetry to be essentially flat (r.m.s. deviation = 0.008 Å); the dihedral angles between it and the two terminal phenyl rings are 69.39 (5) and 59.53 (5)°.

Related literature

For the electronic properties of semiconductors based triarylamines, see, for example: Kennedy *et al.* (2002); Shirota (2000, 2005); Song *et al.* (2006). For the preparation of triarylamine, see: Hartwig (1999). For related structures, see: Kennedy *et al.* (2002); Low *et al.* (2004); Zhang *et al.* (2004, 2006).
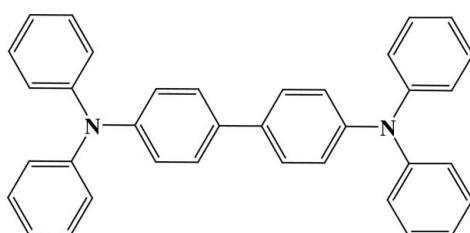
Experimental

Crystal data

$C_{36}H_{28}N_2$

M_r = 488.63

Monoclinic, $P2_1/n$
a = 9.6846 (2) Å
b = 14.2661 (4) Å
c = 9.7946 (2) Å
β = 107.0521 (15)°
V = 1293.75 (5) Å^3

Z = 2
Cu $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 173 K
$0.15 \times 0.14 \times 0.11$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.885, T_{max} = 0.941

14609 measured reflections
2362 independent reflections
1956 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.119
S = 1.07
2362 reflections

174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *CrystalStructure*.

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supporting information

A new crystal phase of *N,N,N′,N′*-tetraphenyl-1,1′-biphenyl-4,4′-diamine

Xiangfeng Shao, Kenshiro Asahi, Takayoshi Yamauchi, Toyonari Sugimoto and Motoo Shiro

S1. Comment

Triarylamine-based organic semiconductors have been intensively investigated as hole transport materials for electro-optic devices (Kennedy *et al.*, 2002; Shirota, 2000; Shirota, 2005). Recently, the organic field-effect transistor (OFET) based on a cyclic triphenylamine has been reported, which shows the relatively good mobility and high on/off ratio (Song *et al.*, 2006). The title compound, *N,N,N′,N′*-tetraphenyl-1,1′-biphenyl-4,4′-diamine (**I**), has been synthesized by coupling of two triphenylamine molecules using a copper catalyst (Ullman coupling) and also using methanesulfonic acid as catalyst in the yield of 10% (Zhang *et al.*, 2006). We have synthesized compound (**I**) from the coupling of 4,4′-dibromo-biphenyl and diphenylamine using a palladium catalyst in the yield of 71% (Hartwig, 1999). The crystal structure of compound (**I**) has been reported (Zhang *et al.*, 2006), where the biphenyl part of the molecule is highly twisted with a dihedral angle of 32.9 (4)°. Herein, we report another crystal phase of compound (**I**).

The molecule (**I**) possesses a inversion center, thus the biphenyl moiety of the molecule shows a completely flat conformation with an average deviation of 0.0079Å (Fig. 1). The other fused rings make 69.39 (5)° and 59.53 (5)° dihedral angles with this flat biphenyl moiety. The N atom displays an almost trigonal geometry with slight distortion of the N—C bond lengths and C—N—C bond angles. The angle sums around the N atom is *ca* 360°. The molecular geometry of (I) is quite different from the previously reported one (Zhang *et al.*, 2006), and also different from those of the related biphenyl-diamine compounds (Kennedy *et al.*, 2002, Low *et al.*, 2004; Zhang *et al.*, 2004). The molecular packing pattern in the present crystal is also different from the reported one (Zhang *et al.*, 2006), and a herringbone-like packing motif governed by the van der Waals interactions is observed (Fig. 2).

S2. Experimental

A suspension of 4,4′-dibromobiphenyl (3.1 g, 10 mmol), diphenylamine (3.9 g, 21 mmol) and sodium *t*-butoxide (2.3 g, 24 mmol) in xylene (20 ml) was refluxed in the presence of palladium(II) acetate (4.4 mg, 0.020 mmol) and triphenyl-phosphine (42 mg, 0.016 mmol) for 5 h under an argon atmosphere. After removing the solvent in vacuum, the residue was separated by column chromatography on silica gel using benzene as eluent to afford the title compound in the yield of 71%. The single crystals of (**I**) suitable for the X-ray crystallographic analysis were obtained by recrystallization from benzene/hexane as colorless blocks.

S3. Refinement

All of the H atoms were positioned geometrically with C–H of 0.95Å and were constrained in a riding motion on their parent carbon atoms with $U_{iso}(H) = 1.2\ U_{eq}(C)$.
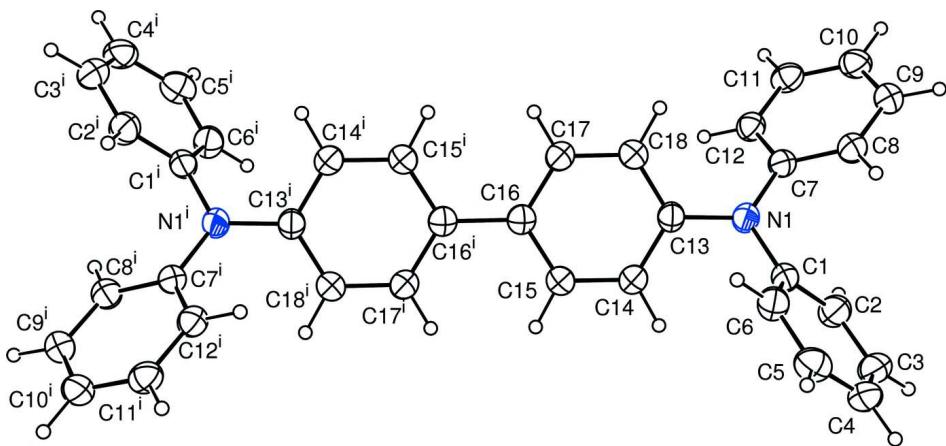
Figure 1

The molecular structure of (**I**), showing 50% probability displacement ellipsoids. [Symmetry code: (i) 1 - *x*, 1 - *y*, -*z*.]
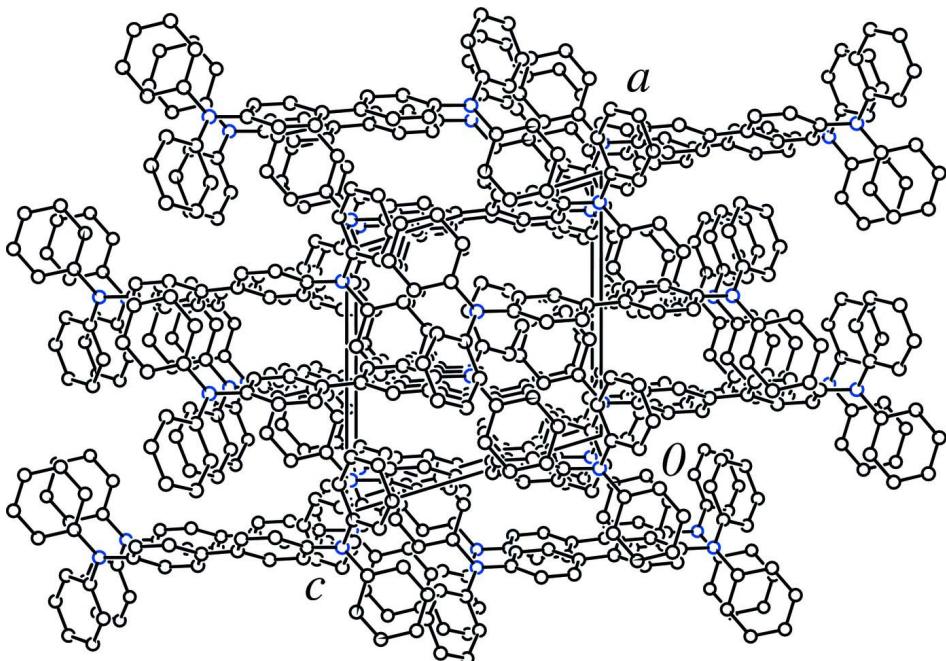
Figure 2

A packing diagram for (**I**), viewed along the *b*-axis. H atoms have been omitted.

N,N,N′,N′-tetraphenyl-1,1′-biphenyl-4,4′-diamine

Crystal data

$C_{36}H_{28}N_2$	$V = 1293.75$ (5) Å^3
$M_r = 488.63$	$Z = 2$
Monoclinic, $P2_1/n$	$F(000) = 516.00$
Hall symbol: -P 2yn	$D_x = 1.254$ Mg m^{-3}
$a = 9.6846$ (2) Å	Melting point: 400 K
$b = 14.2661$ (4) Å	Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å
$c = 9.7946$ (2) Å	Cell parameters from 9402 reflections
$\beta = 107.0521$ (15)°	$\theta = 4.7$–68.2°

$\mu = 0.56$ mm^{-1}	Block, colorless
$T = 173$ K	$0.15 \times 0.14 \times 0.11$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2362 independent reflections
Detector resolution: 10.00 pixels mm^{-1}	1956 reflections with $F^2 > 2\sigma(F^2)$
ω scans	$R_{int} = 0.045$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{max} = 68.2°$
	$h = -11 \rightarrow 11$
$T_{min} = 0.885$, $T_{max} = 0.941$	$k = -17 \rightarrow 16$
14609 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 0.1003P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.119$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2362 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
174 parameters	Extinction correction: *SHELXL97* (Sheldrick, 2008)
0 restraints	
H-atom parameters constrained	Extinction coefficient: 0.0044 (7)

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
N1	0.61552 (11)	0.35882 (8)	0.48812 (11)	0.0350 (3)
C1	0.75255 (14)	0.38277 (9)	0.58558 (13)	0.0322 (3)
C2	0.76352 (16)	0.41058 (10)	0.72442 (14)	0.0407 (3)
C3	0.89748 (16)	0.43064 (10)	0.81905 (15)	0.0460 (4)
C4	1.02051 (16)	0.42680 (10)	0.77599 (16)	0.0435 (3)
C5	1.00977 (15)	0.40187 (10)	0.63705 (16)	0.0419 (3)
C6	0.87666 (15)	0.37871 (9)	0.54238 (15)	0.0375 (3)
C7	0.52193 (14)	0.29751 (9)	0.53277 (13)	0.0312 (3)
C8	0.57988 (15)	0.22955 (9)	0.63602 (13)	0.0364 (3)
C9	0.49026 (15)	0.17243 (10)	0.68654 (14)	0.0408 (3)
C10	0.34163 (15)	0.17989 (10)	0.63263 (14)	0.0406 (3)
C11	0.28345 (15)	0.24546 (10)	0.52752 (14)	0.0370 (3)
C12	0.37225 (14)	0.30446 (9)	0.47834 (13)	0.0329 (3)
C13	0.57704 (13)	0.39859 (9)	0.34918 (13)	0.0303 (3)
C14	0.61838 (14)	0.48974 (9)	0.33017 (13)	0.0333 (3)
C15	0.58792 (14)	0.52884 (9)	0.19522 (13)	0.0322 (3)
C16	0.51417 (12)	0.47929 (9)	0.07275 (12)	0.0286 (3)
C17	0.46985 (14)	0.38858 (9)	0.09424 (13)	0.0338 (3)
C18	0.50099 (14)	0.34835 (9)	0.22831 (13)	0.0344 (3)

H2	0.6790	0.4158	0.7544	0.049*
H3	0.9045	0.4473	0.9148	0.055*
H4	1.1119	0.4412	0.8413	0.052*
H5	1.0939	0.4006	0.6060	0.050*
H6	0.8706	0.3600	0.4477	0.045*
H8	0.6817	0.2224	0.6719	0.044*
H9	0.5311	0.1277	0.7589	0.049*
H10	0.2804	0.1405	0.6674	0.049*
H11	0.1816	0.2501	0.4886	0.044*
H12	0.3308	0.3498	0.4072	0.039*
H14	0.6684	0.5258	0.4111	0.040*
H15	0.6181	0.5912	0.1857	0.039*
H17	0.4164	0.3533	0.0138	0.041*
H18	0.4704	0.2861	0.2382	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0320 (6)	0.0420 (6)	0.0280 (5)	−0.0078 (4)	0.0041 (4)	0.0056 (4)
C1	0.0307 (7)	0.0328 (7)	0.0304 (6)	−0.0044 (5)	0.0049 (5)	0.0059 (4)
C2	0.0374 (7)	0.0514 (8)	0.0347 (7)	−0.0094 (6)	0.0125 (6)	−0.0006 (6)
C3	0.0506 (9)	0.0517 (9)	0.0323 (7)	−0.0171 (7)	0.0066 (6)	−0.0038 (6)
C4	0.0349 (7)	0.0412 (8)	0.0461 (8)	−0.0087 (6)	−0.0010 (6)	0.0025 (6)
C5	0.0311 (7)	0.0400 (7)	0.0550 (9)	0.0004 (5)	0.0132 (6)	0.0030 (6)
C6	0.0370 (8)	0.0406 (7)	0.0343 (7)	0.0005 (5)	0.0097 (5)	0.0019 (5)
C7	0.0328 (7)	0.0333 (7)	0.0272 (6)	−0.0060 (5)	0.0083 (5)	−0.0003 (4)
C8	0.0328 (7)	0.0389 (7)	0.0342 (7)	−0.0043 (5)	0.0047 (5)	0.0034 (5)
C9	0.0468 (8)	0.0386 (7)	0.0339 (7)	−0.0088 (6)	0.0069 (6)	0.0057 (5)
C10	0.0450 (8)	0.0430 (8)	0.0365 (7)	−0.0138 (6)	0.0162 (6)	−0.0024 (5)
C11	0.0315 (7)	0.0451 (8)	0.0354 (7)	−0.0055 (5)	0.0112 (5)	−0.0064 (5)
C12	0.0342 (7)	0.0346 (7)	0.0295 (6)	−0.0010 (5)	0.0086 (5)	−0.0015 (5)
C13	0.0280 (6)	0.0353 (7)	0.0273 (6)	0.0001 (5)	0.0078 (5)	0.0038 (4)
C14	0.0353 (7)	0.0330 (7)	0.0290 (6)	−0.0020 (5)	0.0052 (5)	−0.0014 (5)
C15	0.0345 (7)	0.0287 (6)	0.0323 (6)	−0.0013 (5)	0.0081 (5)	0.0014 (4)
C16	0.0231 (6)	0.0322 (6)	0.0307 (6)	0.0034 (4)	0.0081 (5)	0.0015 (4)
C17	0.0346 (7)	0.0367 (7)	0.0284 (6)	−0.0051 (5)	0.0064 (5)	−0.0012 (5)
C18	0.0375 (7)	0.0324 (7)	0.0328 (6)	−0.0060 (5)	0.0096 (5)	0.0021 (5)

Geometric parameters (Å, º)

N1—C1	1.4304 (14)	C15—C16	1.3951 (16)
N1—C7	1.4178 (18)	C16—C16ⁱ	1.4920 (16)
N1—C13	1.4196 (16)	C16—C17	1.3986 (18)
C1—C2	1.3904 (19)	C17—C18	1.3829 (17)
C1—C6	1.388 (2)	C2—H2	0.950
C2—C3	1.3852 (18)	C3—H3	0.950
C3—C4	1.377 (2)	C4—H4	0.950
C4—C5	1.381 (2)	C5—H5	0.950

C5—C6	1.3892 (17)	C6—H6	0.950
C7—C8	1.3946 (17)	C8—H8	0.950
C7—C12	1.3936 (17)	C9—H9	0.950
C8—C9	1.384 (2)	C10—H10	0.950
C9—C10	1.3843 (19)	C11—H11	0.950
C10—C11	1.3828 (18)	C12—H12	0.950
C11—C12	1.387 (2)	C14—H14	0.950
C13—C14	1.3891 (18)	C15—H15	0.950
C13—C18	1.3951 (16)	C17—H17	0.950
C14—C15	1.3844 (17)	C18—H18	0.950
C4···C9ii	3.528 (2)	C14···H5vi	3.095
C12···C14iii	3.4707 (18)	C14···H10viii	3.150
N1···H14iii	3.582	C14···H12iii	3.370
C1···H18iv	3.262	C15···H2iii	2.881
C2···H18iv	3.427	C15···H4vi	3.061
C3···H3v	3.252	C15···H5vi	3.283
C3···H9ii	3.045	C15···H10viii	3.111
C3···H18iv	3.319	C16···H2iii	3.235
C4···H3v	3.412	C16···H10viii	3.004
C4···H9ii	2.912	C17···H8ix	3.482
C4···H10ii	3.562	C17···H10viii	2.910
C4···H15vi	3.418	C17···H11viii	3.230
C4···H18iv	3.081	C18···H8ix	3.144
C5···H9ii	3.436	C18···H10viii	2.941
C5···H11vii	3.315	C18···H11viii	3.599
C5···H14vi	3.445	H2···H11iv	3.291
C5···H15vi	3.513	H2···H14iii	3.382
C5···H18iv	2.922	H2···H15iii	3.102
C6···H5vi	3.515	H3···H3v	2.581
C6···H9viii	3.520	H3···H4v	2.914
C6···H10viii	3.525	H3···H9ii	3.245
C6···H17iv	3.353	H3···H9iv	3.404
C6···H18iv	3.001	H3···H10iv	3.298
C7···H14iii	3.263	H4···H9ii	3.027
C8···H3ix	3.433	H4···H10ii	3.038
C8···H11iv	3.314	H4···H15vi	2.743
C8···H12iv	3.234	H4···H17xiii	3.194
C9···H3x	3.597	H4···H18iv	3.549
C9···H3ix	3.065	H5···H6vi	3.488
C9···H4x	3.432	H5···H9viii	3.298
C9···H6xi	3.137	H5···H11vii	2.687
C9···H11iv	3.192	H5···H12vii	3.493
C9···H12iv	3.387	H5···H14vi	2.580
C10···H3ix	2.996	H5···H15vi	2.935
C10···H4x	3.435	H5···H18iv	3.332
C10···H6xi	3.069	H6···H9viii	2.748
C11···H2ix	3.447	H6···H10viii	2.626

C11···H3ⁱˣ	3.303	H6···H11ᵛⁱⁱ	3.314
C11···H5ˣⁱⁱ	3.112	H6···H17ⁱᵛ	3.116
C11···H8ⁱˣ	3.361	H6···H18ⁱᵛ	3.429
C11···H9ⁱˣ	3.521	H8···H11ⁱᵛ	3.127
C11···H14ⁱⁱⁱ	3.326	H8···H12ⁱᵛ	2.551
C11···H15ⁱⁱⁱ	3.557	H8···H17ⁱᵛ	3.286
C12···H5ˣⁱⁱ	3.562	H8···H18ⁱᵛ	2.682
C12···H8ⁱˣ	3.052	H9···H11ⁱᵛ	2.881
C12···H9ⁱˣ	3.508	H9···H12ⁱᵛ	2.857
C12···H14ⁱⁱⁱ	2.728	H10···H17ˣⁱ	3.404
C12···H15ⁱⁱⁱ	3.587	H10···H18ˣⁱ	3.437
C13···H2ⁱⁱⁱ	3.566	H11···H14ⁱⁱⁱ	3.529
C13···H10ᵛⁱⁱⁱ	3.068	H11···H17ˣⁱ	3.034
C14···H2ⁱⁱⁱ	3.066	H12···H14ⁱⁱⁱ	2.511
C1—N1—C7	119.56 (10)	C1—C2—H2	120.0
C1—N1—C13	118.40 (10)	C3—C2—H2	120.0
C7—N1—C13	122.03 (9)	C2—C3—H3	119.6
N1—C1—C2	120.71 (13)	C4—C3—H3	119.6
N1—C1—C6	120.24 (11)	C3—C4—H4	120.3
C2—C1—C6	119.05 (11)	C5—C4—H4	120.3
C1—C2—C3	120.09 (14)	C4—C5—H5	119.8
C2—C3—C4	120.78 (13)	C6—C5—H5	119.8
C3—C4—C5	119.37 (12)	C1—C6—H6	119.9
C4—C5—C6	120.41 (15)	C5—C6—H6	119.9
C1—C6—C5	120.25 (13)	C7—C8—H8	119.7
N1—C7—C8	119.66 (11)	C9—C8—H8	119.8
N1—C7—C12	121.70 (10)	C8—C9—H9	119.7
C8—C7—C12	118.63 (12)	C10—C9—H9	119.7
C7—C8—C9	120.50 (12)	C9—C10—H10	120.4
C8—C9—C10	120.63 (12)	C11—C10—H10	120.4
C9—C10—C11	119.15 (14)	C10—C11—H11	119.7
C10—C11—C12	120.69 (12)	C12—C11—H11	119.7
C7—C12—C11	120.36 (11)	C7—C12—H12	119.8
N1—C13—C14	119.85 (10)	C11—C12—H12	119.8
N1—C13—C18	122.21 (11)	C13—C14—H14	119.5
C14—C13—C18	117.93 (11)	C15—C14—H14	119.5
C13—C14—C15	121.07 (10)	C14—C15—H15	119.0
C14—C15—C16	121.92 (11)	C16—C15—H15	119.0
C15—C16—C16ⁱ	121.67 (11)	C16—C17—H17	118.8
C15—C16—C17	116.22 (10)	C18—C17—H17	118.8
C16ⁱ—C16—C17	122.11 (10)	C13—C18—H18	119.8
C16—C17—C18	122.40 (10)	C17—C18—H18	119.8
C13—C18—C17	120.43 (11)		
C(1)—N(1)—C(7)—C(8)	−29.27 (18)	N(1)—C(7)—C(8)—C(9)	176.51 (12)
C(1)—N(1)—C(7)—C(12)	149.31 (12)	N(1)—C(7)—C(12)—C(11)	−177.89 (12)
C(7)—N(1)—C(1)—C(2)	−47.50 (17)	C(8)—C(7)—C(12)—C(11)	0.71 (19)

C(7)—N(1)—C(1)—C(6)	132.65 (13)	C(12)—C(7)—C(8)—C(9)	−2.12 (19)
C(1)—N(1)—C(13)—C(14)	−35.87 (18)	C(7)—C(8)—C(9)—C(10)	1.9 (2)
C(1)—N(1)—C(13)—C(18)	142.58 (13)	C(8)—C(9)—C(10)—C(11)	−0.1 (2)
C(13)—N(1)—C(1)—C(2)	131.78 (13)	C(9)—C(10)—C(11)—C(12)	−1.3 (2)
C(13)—N(1)—C(1)—C(6)	−48.07 (17)	C(10)—C(11)—C(12)—C(7)	1.0 (2)
C(7)—N(1)—C(13)—C(14)	143.40 (13)	N(1)—C(13)—C(14)—C(15)	177.10 (12)
C(7)—N(1)—C(13)—C(18)	−38.16 (19)	N(1)—C(13)—C(18)—C(17)	−177.79 (12)
C(13)—N(1)—C(7)—C(8)	151.47 (12)	C(14)—C(13)—C(18)—C(17)	0.7 (2)
C(13)—N(1)—C(7)—C(12)	−29.94 (18)	C(18)—C(13)—C(14)—C(15)	−1.4 (2)
N(1)—C(1)—C(2)—C(3)	177.90 (12)	C(13)—C(14)—C(15)—C(16)	0.4 (2)
N(1)—C(1)—C(6)—C(5)	−179.93 (12)	C(14)—C(15)—C(16)—C(17)	1.39 (19)
C(2)—C(1)—C(6)—C(5)	0.21 (19)	C(14)—C(15)—C(16)—C(16)^i	−178.00 (12)
C(6)—C(1)—C(2)—C(3)	−2.2 (2)	C(15)—C(16)—C(16)^i—C(17)^i	−0.65 (19)
C(1)—C(2)—C(3)—C(4)	2.4 (2)	C(15)—C(16)—C(17)—C(18)	−2.1 (2)
C(2)—C(3)—C(4)—C(5)	−0.5 (2)	C(16)^i—C(16)—C(17)—C(18)	177.25 (12)
C(3)—C(4)—C(5)—C(6)	−1.5 (2)	C(17)—C(16)—C(16)^i—C(15)^i	0.65 (19)
C(4)—C(5)—C(6)—C(1)	1.7 (2)	C(16)—C(17)—C(18)—C(13)	1.1 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (v) −*x*+2, −*y*+1, −*z*+2; (vi) −*x*+2, −*y*+1, −*z*+1; (vii) *x*+1, *y*, *z*; (viii) *x*+1/2, −*y*+1/2, *z*−1/2; (ix) *x*−1/2, −*y*+1/2, *z*−1/2; (x) −*x*+3/2, *y*−1/2, −*z*+3/2; (xi) *x*−1/2, −*y*+1/2, *z*+1/2; (xii) *x*−1, *y*, *z*; (xiii) *x*+1, *y*, *z*+1.