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2-[3-(Naphthalen-2-yl)phenyl]naphthalene[1]

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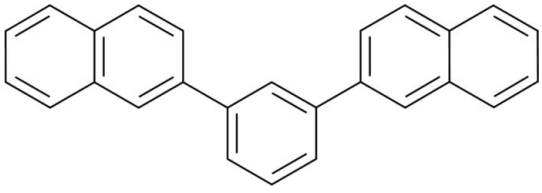
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.045; wR factor = 0.125; data-to-parameter ratio = 21.6.

The title compound, $C_{26}H_{18}$, consists of a benzene ring with *meta*-substituted 2-naphthalene substituents, which are essentially planar [r.m.s. deviations = 0.022 (1) and 0.003 (1) Å]. The conformation is *syn*, with equivalent torsion angles about the benzene–naphthalene bonds of −36.04 (13) and +34.14 (13)°. The molecule has quasi-C_s molecular symmetry.

Related literature

For properties of oligophenyls, see: Bocchinfuso *et al.* (2009) and for their synthesis, see: Marcinow & Rabideau (1990); Du *et al.* (1986); Woods *et al.* (1951). For similar structures, see: Baker *et al.* (1990); Lin & Williams (1975); Bart (1968); Tummala *et al.* (2013). For conformational calculations with *GAUSSIAN09*, see: Frisch *et al.* (2009).



Experimental

Crystal data

$C_{26}H_{18}$
M_r = 330.4
Orthorhombic, *Pbcn*
a = 25.9304 (3) Å
b = 8.9300 (1) Å
c = 14.9377 (2) Å
V = 3458.95 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100 K
0.40 × 0.27 × 0.22 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.972, T_{max} = 0.984
37425 measured reflections
6240 independent reflections
4993 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.02
6240 reflections
289 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *COLLECT* (Nonius 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

The purchase of the diffractometer was made possible by grant No. LEQSF(1999–2000)-ESH-TR-13, administered by the Louisiana Board of Regents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2619).

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2-[3-(Naphthalen-2-yl)phenyl]naphthalene

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S1. Comment

The crystal and molecular structures of *p*-oligophenyls have been well investigated (Baker *et al.*, 1990, and references therein), but relatively few studies have appeared concerning the conformational preferences of *m*-oligophenyls. Two interesting papers were reported, one by Lin & Williams (1975) about the crystal structure of 1,3,5 triphenyl, which serves as a model for *m*-polyphenyls, showing substituted phenyl groups being twisted about the formal single bonds by +40.7, -37.2, and +36.1° out of the plane of the central ring. The crystal structure of one of the polymorphic forms of hexaphenyl benzene, reported by Bart (1968), has shown that the peripheral rings are not perpendicular to the central ring, but are twisted by about 25°. The molecule was found to be highly distorted as a result of out-of-plane bending of the exocyclic bonds. Therefore, we have studied the structure of 1,3-bis(2-naphthyl)benzene for comparison of its conformation with the previous results.

Title compound **I** is of quasi-C_s symmetry and consists of a benzene ring with *meta*-substituted 2-naphthalenes. The benzene ring is nearly planar (C-atoms only, $\delta_{r.m.s.}$ = 0.005 (1) Å), as are the two naphthalenes ($\delta_{r.m.s.}$ = 0.022 (1) and 0.003 (1) Å). The benzene plane and both naphthalene planes are bent with respect to the benzene-naphthalene (BN) bonds: C8 and C18 lie above the benzene plane by 0.039 (2) and 0.040 (1) Å respectively, while C1 lies above its proximate naphthalene plane by 0.016 (1) Å, and C3 lies above its proximate naphthalene plane by 0.085 (1) Å. The naphthalene ring planes are also twisted about the BN bonds with equivalent torsion angles of -36.04 (13)° (C6–C1–C8–C7) and +34.14 (13)° (C4–C3–C18–C17). An isolated and optimized C_s model (Gaussian09; Frisch *et al.*, 2009; DFT:b3lyp/3–21 g) shows a small amount of bending about the BN bonds, with equivalent distances from mean planes C8/C18 = 0.020 Å and C1/C3 = 0.004 Å, and BN torsion angles of ± 43°.

S2. Experimental

Compound **I** was prepared after Du *et al.* (1986) and recrystallized from petroleum ether.

S3. Refinement

The positional parameters of all H atoms were refined, but U_{iso}(H) was set to 1.2U_{eq} of the attached C atom. The range of C–H distances is 0.959 (14) - 1.020 (14) Å.

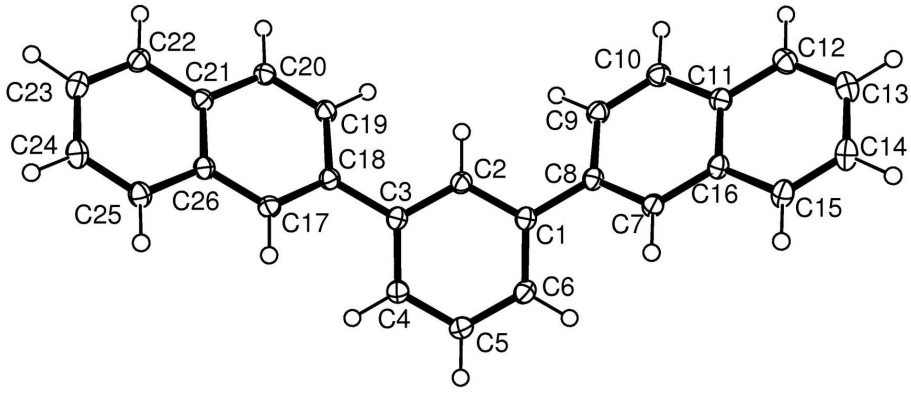

Figure 1

View of (I) (50% probability displacement ellipsoids)

2-[3-(Naphthalen-2-yl)phenyl]naphthalene

Crystal data

$C_{26}H_{18}$
M_r = 330.4
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
a = 25.9304 (3) Å
b = 8.9300 (1) Å
c = 14.9377 (2) Å
V = 3458.95 (7) Å^3
Z = 8
F(000) = 1392
D_x = 1.269 Mg m^{-3}
Melting point: 143.5(5) K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6568 reflections
θ = 2.6–32.6°
μ = 0.07 mm^{-1}
T = 100 K
Prism, colourless
0.40 × 0.27 × 0.22 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.972, T_{max} = 0.984
37425 measured reflections
6240 independent reflections
4993 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 32.6°, θ_{min} = 2.7°
h = −39→39
k = −13→13
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.02
6240 reflections
289 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.9158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.63414 (3)	0.65124 (10)	0.39203 (6)	0.01689 (17)
C2	0.62992 (3)	0.71392 (10)	0.30628 (6)	0.01694 (16)
H2	0.6484 (5)	0.8056 (15)	0.2934 (8)	0.02*
C3	0.59837 (3)	0.65068 (10)	0.24032 (6)	0.01660 (16)
C4	0.57139 (4)	0.51927 (11)	0.26073 (6)	0.01896 (17)
H4	0.5494 (5)	0.4704 (15)	0.2136 (8)	0.023*
C5	0.57577 (4)	0.45461 (11)	0.34519 (6)	0.02072 (18)
H5	0.5574 (5)	0.3638 (16)	0.3575 (8)	0.025*
C6	0.60671 (4)	0.51962 (11)	0.41055 (6)	0.01975 (18)
H6	0.6101 (5)	0.4717 (15)	0.4700 (9)	0.024*
C7	0.65216 (4)	0.72652 (11)	0.55034 (6)	0.01811 (17)
H7	0.6193 (5)	0.6799 (15)	0.5698 (8)	0.022*
C8	0.66657 (3)	0.72466 (10)	0.46121 (6)	0.01701 (16)
C9	0.71347 (4)	0.79654 (11)	0.43622 (6)	0.01953 (17)
H9	0.7242 (5)	0.7931 (15)	0.3721 (8)	0.023*
C10	0.74404 (4)	0.86589 (11)	0.49847 (6)	0.02031 (18)
H10	0.7772 (5)	0.9160 (15)	0.4807 (8)	0.024*
C11	0.72952 (4)	0.86948 (10)	0.59028 (6)	0.01801 (17)
C12	0.76011 (4)	0.94138 (11)	0.65616 (7)	0.02206 (19)
H12	0.7930 (5)	0.9933 (16)	0.6373 (9)	0.026*
C13	0.74530 (4)	0.94171 (12)	0.74436 (7)	0.0246 (2)
H13	0.7680 (5)	0.9909 (16)	0.7903 (9)	0.03*
C14	0.69902 (4)	0.87049 (13)	0.77044 (6)	0.0248 (2)
H14	0.6888 (5)	0.8669 (17)	0.8349 (9)	0.03*
C15	0.66831 (4)	0.80109 (12)	0.70813 (6)	0.02236 (19)
H15	0.6365 (5)	0.7517 (16)	0.7256 (9)	0.027*
C16	0.68280 (4)	0.79842 (10)	0.61631 (6)	0.01787 (17)
C17	0.54718 (3)	0.72005 (10)	0.10483 (6)	0.01746 (17)
H17	0.5158 (5)	0.6693 (15)	0.1293 (8)	0.021*
C18	0.59332 (3)	0.72319 (10)	0.15125 (6)	0.01630 (16)
C19	0.63624 (3)	0.79954 (11)	0.11308 (6)	0.01800 (17)
H19	0.6705 (5)	0.8014 (15)	0.1453 (8)	0.022*
C20	0.63221 (3)	0.86852 (11)	0.03141 (6)	0.01788 (17)
H20	0.6622 (5)	0.9217 (15)	0.0055 (8)	0.021*
C21	0.58490 (3)	0.86835 (10)	−0.01638 (6)	0.01625 (16)
C22	0.57913 (4)	0.94470 (11)	−0.09892 (6)	0.01963 (18)
H22	0.6099 (5)	0.9976 (15)	−0.1227 (9)	0.024*
C23	0.53253 (4)	0.94754 (12)	−0.14213 (6)	0.02269 (19)
H23	0.5289 (5)	1.0075 (16)	−0.1999 (9)	0.027*

C24	0.48948 (4)	0.87247 (12)	−0.10533 (6)	0.02300 (19)
H24	0.4556 (5)	0.8770 (16)	−0.1362 (9)	0.028*
C25	0.49393 (4)	0.79656 (11)	−0.02576 (6)	0.02032 (18)
H25	0.4636 (5)	0.7474 (16)	0.0014 (8)	0.024*
C26	0.54175 (3)	0.79277 (10)	0.02090 (6)	0.01655 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0171 (4)	0.0180 (4)	0.0155 (4)	0.0020 (3)	0.0003 (3)	−0.0006 (3)
C2	0.0186 (4)	0.0168 (4)	0.0154 (4)	0.0002 (3)	0.0008 (3)	0.0003 (3)
C3	0.0170 (4)	0.0177 (4)	0.0151 (3)	0.0020 (3)	0.0006 (3)	−0.0004 (3)
C4	0.0204 (4)	0.0185 (4)	0.0180 (4)	−0.0005 (3)	−0.0009 (3)	0.0001 (3)
C5	0.0237 (4)	0.0183 (4)	0.0202 (4)	−0.0023 (3)	−0.0001 (3)	0.0023 (3)
C6	0.0232 (4)	0.0189 (4)	0.0172 (4)	0.0007 (3)	0.0001 (3)	0.0028 (3)
C7	0.0170 (4)	0.0212 (4)	0.0161 (4)	−0.0001 (3)	−0.0001 (3)	0.0021 (3)
C8	0.0179 (4)	0.0172 (4)	0.0159 (4)	0.0016 (3)	−0.0009 (3)	0.0010 (3)
C9	0.0195 (4)	0.0220 (4)	0.0171 (4)	−0.0002 (3)	0.0018 (3)	0.0009 (3)
C10	0.0186 (4)	0.0221 (4)	0.0202 (4)	−0.0011 (3)	0.0012 (3)	0.0015 (3)
C11	0.0171 (4)	0.0182 (4)	0.0187 (4)	0.0019 (3)	−0.0011 (3)	0.0009 (3)
C12	0.0209 (4)	0.0212 (4)	0.0241 (4)	0.0006 (3)	−0.0031 (3)	−0.0015 (3)
C13	0.0251 (5)	0.0265 (5)	0.0224 (4)	0.0049 (4)	−0.0058 (4)	−0.0052 (4)
C14	0.0256 (5)	0.0319 (5)	0.0169 (4)	0.0058 (4)	−0.0019 (3)	−0.0024 (4)
C15	0.0218 (4)	0.0288 (5)	0.0165 (4)	0.0020 (4)	0.0005 (3)	0.0010 (3)
C16	0.0175 (4)	0.0205 (4)	0.0156 (4)	0.0022 (3)	−0.0013 (3)	0.0011 (3)
C17	0.0168 (4)	0.0187 (4)	0.0169 (4)	−0.0013 (3)	0.0012 (3)	0.0002 (3)
C18	0.0181 (4)	0.0161 (4)	0.0146 (3)	−0.0001 (3)	0.0004 (3)	−0.0010 (3)
C19	0.0161 (4)	0.0211 (4)	0.0168 (4)	−0.0011 (3)	−0.0007 (3)	−0.0007 (3)
C20	0.0175 (4)	0.0193 (4)	0.0168 (4)	−0.0024 (3)	0.0004 (3)	−0.0003 (3)
C21	0.0179 (4)	0.0157 (4)	0.0152 (4)	0.0001 (3)	0.0000 (3)	−0.0016 (3)
C22	0.0235 (4)	0.0189 (4)	0.0165 (4)	0.0001 (3)	0.0009 (3)	0.0011 (3)
C23	0.0271 (5)	0.0234 (4)	0.0176 (4)	0.0038 (4)	−0.0022 (3)	0.0019 (3)
C24	0.0208 (4)	0.0269 (5)	0.0213 (4)	0.0036 (4)	−0.0047 (3)	−0.0001 (4)
C25	0.0173 (4)	0.0235 (4)	0.0201 (4)	0.0008 (3)	−0.0014 (3)	−0.0009 (3)
C26	0.0170 (4)	0.0172 (4)	0.0154 (4)	0.0009 (3)	0.0000 (3)	−0.0013 (3)

Geometric parameters (Å, º)

C1—C6	1.4014 (13)	C13—C14	1.4129 (16)
C1—C2	1.4022 (12)	C13—H13	1.005 (14)
C1—C8	1.4850 (12)	C14—C15	1.3729 (14)
C2—C3	1.3995 (12)	C14—H14	0.999 (13)
C2—H2	0.968 (13)	C15—C16	1.4224 (13)
C3—C4	1.3999 (13)	C15—H15	0.970 (14)
C3—C18	1.4856 (12)	C17—C18	1.3830 (12)
C4—C5	1.3922 (13)	C17—C26	1.4190 (12)
C4—H4	1.005 (13)	C17—H17	1.000 (13)
C5—C6	1.3907 (13)	C18—C19	1.4243 (12)

C5—H5	0.959 (14)	C19—C20	1.3707 (12)
C6—H6	0.989 (13)	C19—H19	1.012 (13)
C7—C8	1.3829 (12)	C20—C21	1.4193 (12)
C7—C16	1.4193 (13)	C20—H20	0.990 (13)
C7—H7	0.991 (13)	C21—C22	1.4168 (12)
C8—C9	1.4250 (13)	C21—C26	1.4204 (12)
C9—C10	1.3698 (13)	C22—C23	1.3702 (14)
C9—H9	0.997 (13)	C22—H22	0.994 (13)
C10—C11	1.4226 (13)	C23—C24	1.4136 (14)
C10—H10	1.006 (13)	C23—H23	1.020 (14)
C11—C12	1.4178 (13)	C24—C25	1.3731 (13)
C11—C16	1.4217 (13)	C24—H24	0.992 (13)
C12—C13	1.3723 (14)	C25—C26	1.4229 (13)
C12—H12	1.010 (13)	C25—H25	0.987 (13)

C6—C1—C2	118.39 (8)	C15—C14—C13	120.59 (9)
C6—C1—C8	121.35 (8)	C15—C14—H14	118.9 (8)
C2—C1—C8	120.25 (8)	C13—C14—H14	120.4 (8)
C3—C2—C1	121.85 (8)	C14—C15—C16	120.54 (9)
C3—C2—H2	119.4 (7)	C14—C15—H15	121.1 (8)
C1—C2—H2	118.7 (7)	C16—C15—H15	118.4 (8)
C2—C3—C4	118.50 (8)	C7—C16—C11	119.27 (8)
C2—C3—C18	120.41 (8)	C7—C16—C15	121.95 (9)
C4—C3—C18	121.08 (8)	C11—C16—C15	118.78 (8)
C5—C4—C3	120.28 (8)	C18—C17—C26	121.30 (8)
C5—C4—H4	120.1 (7)	C18—C17—H17	121.9 (7)
C3—C4—H4	119.7 (7)	C26—C17—H17	116.7 (7)
C6—C5—C4	120.68 (9)	C17—C18—C19	119.01 (8)
C6—C5—H5	120.4 (8)	C17—C18—C3	121.10 (8)
C4—C5—H5	119.0 (8)	C19—C18—C3	119.88 (8)
C5—C6—C1	120.28 (8)	C20—C19—C18	120.78 (8)
C5—C6—H6	120.0 (8)	C20—C19—H19	118.9 (7)
C1—C6—H6	119.7 (8)	C18—C19—H19	120.3 (7)
C8—C7—C16	121.51 (9)	C19—C20—C21	120.87 (8)
C8—C7—H7	120.6 (7)	C19—C20—H20	120.2 (7)
C16—C7—H7	117.9 (7)	C21—C20—H20	118.9 (7)
C7—C8—C9	118.52 (8)	C22—C21—C20	121.90 (8)
C7—C8—C1	121.48 (8)	C22—C21—C26	119.12 (8)
C9—C8—C1	120.00 (8)	C20—C21—C26	118.96 (8)
C10—C9—C8	121.31 (8)	C23—C22—C21	120.80 (9)
C10—C9—H9	120.3 (8)	C23—C22—H22	122.1 (7)
C8—C9—H9	118.4 (8)	C21—C22—H22	117.1 (7)
C9—C10—C11	120.75 (9)	C22—C23—C24	120.30 (9)
C9—C10—H10	121.1 (7)	C22—C23—H23	119.3 (7)
C11—C10—H10	118.1 (7)	C24—C23—H23	120.4 (7)
C12—C11—C16	119.28 (8)	C25—C24—C23	120.29 (9)
C12—C11—C10	122.08 (9)	C25—C24—H24	119.8 (8)
C16—C11—C10	118.64 (8)	C23—C24—H24	119.9 (8)

C13—C12—C11	120.71 (9)	C24—C25—C26	120.60 (9)
C13—C12—H12	120.2 (8)	C24—C25—H25	120.5 (8)
C11—C12—H12	119.1 (8)	C26—C25—H25	118.8 (8)
C12—C13—C14	120.10 (9)	C17—C26—C21	119.06 (8)
C12—C13—H13	119.4 (8)	C17—C26—C25	122.01 (8)
C14—C13—H13	120.4 (8)	C21—C26—C25	118.89 (8)

C6—C1—C2—C3	1.51 (13)	C10—C11—C16—C7	−0.07 (13)
C8—C1—C2—C3	−177.83 (8)	C12—C11—C16—C15	−0.31 (13)
C1—C2—C3—C4	−1.46 (13)	C10—C11—C16—C15	179.66 (9)
C1—C2—C3—C18	177.73 (8)	C14—C15—C16—C7	179.43 (9)
C2—C3—C4—C5	0.54 (13)	C14—C15—C16—C11	−0.28 (15)
C18—C3—C4—C5	−178.65 (9)	C26—C17—C18—C19	−0.81 (14)
C3—C4—C5—C6	0.30 (14)	C26—C17—C18—C3	178.19 (8)
C4—C5—C6—C1	−0.24 (15)	C2—C3—C18—C17	−145.04 (9)
C2—C1—C6—C5	−0.64 (14)	C4—C3—C18—C17	34.14 (13)
C8—C1—C6—C5	178.69 (9)	C2—C3—C18—C19	33.95 (12)
C16—C7—C8—C9	0.27 (14)	C4—C3—C18—C19	−146.87 (9)
C16—C7—C8—C1	−179.14 (8)	C17—C18—C19—C20	−0.30 (14)
C6—C1—C8—C7	−36.04 (13)	C3—C18—C19—C20	−179.31 (8)
C2—C1—C8—C7	143.28 (9)	C18—C19—C20—C21	1.32 (14)
C6—C1—C8—C9	144.56 (9)	C19—C20—C21—C22	177.04 (9)
C2—C1—C8—C9	−36.12 (13)	C19—C20—C21—C26	−1.24 (14)
C7—C8—C9—C10	0.22 (14)	C20—C21—C22—C23	−177.55 (9)
C1—C8—C9—C10	179.64 (9)	C26—C21—C22—C23	0.72 (14)
C8—C9—C10—C11	−0.64 (15)	C21—C22—C23—C24	−0.75 (15)
C9—C10—C11—C12	−179.48 (9)	C22—C23—C24—C25	0.27 (15)
C9—C10—C11—C16	0.55 (14)	C23—C24—C25—C26	0.23 (15)
C16—C11—C12—C13	0.59 (14)	C18—C17—C26—C21	0.87 (13)
C10—C11—C12—C13	−179.38 (9)	C18—C17—C26—C25	−177.02 (9)
C11—C12—C13—C14	−0.27 (15)	C22—C21—C26—C17	−178.18 (8)
C12—C13—C14—C15	−0.34 (16)	C20—C21—C26—C17	0.15 (13)
C13—C14—C15—C16	0.61 (16)	C22—C21—C26—C25	−0.22 (13)
C8—C7—C16—C11	−0.34 (14)	C20—C21—C26—C25	178.10 (8)
C8—C7—C16—C15	179.94 (9)	C24—C25—C26—C17	177.64 (9)
C12—C11—C16—C7	179.96 (9)	C24—C25—C26—C21	−0.25 (14)