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N-(9*H*-Fluoren-9-ylidene)-4-methylaniline

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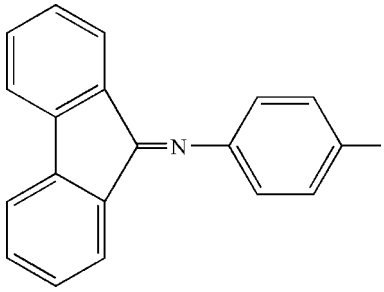
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.115; data-to-parameter ratio = 14.1.

In the title compound, $C_{20}H_{15}N$, the fluorene unit is essentially planar [r.m.s. deviation 0.0334 Å] and the benzene ring bound to the imine N atom bears a methyl group which is nearly coplanar [dihedral angle 0.5 (1)°]. The dihedral angle between the substituent benzene ring and the 9*H*-fluoren-9-imine unit is 71.1 (3)°. Intermolecular π–π interactions between the benzene rings of adjacent fluorene units [centroid–centroid distance 3.8081 (13) Å] are present in the crystal structure, resulting in a one-dimensional supramolecular architecture.

Related literature

For the properties of Schiff bases, see: Xu *et al.* (2007); Tanaka *et al.* (2006). For the properties of fluorene derivatives, see: Saragi *et al.* (2004). For related structures, see: Glagovich *et al.* (2004); Peters *et al.* (1998); Pierre *et al.* (1997).



Experimental

Crystal data

$C_{20}H_{15}N$
M_r = 269.33
Monoclinic, $P2_1/n$
a = 5.6423 (10) Å
b = 12.187 (2) Å
c = 21.310 (4) Å
β = 94.441 (2)°
V = 1460.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 294 K
0.35 × 0.17 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.994
10793 measured reflections
2711 independent reflections
1779 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.01
2711 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2179).

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supporting information

Acta Cryst. (2009). E**65**, o1545 [doi:10.1107/S1600536809020765]

N-(9*H*-Fluoren-9-ylidene)-4-methylaniline

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S1. Comment

Schiff bases have received much attention during the past decades because of their strong coordination capability and diverse biological activities (Xu *et al.*, 2007; Tanaka *et al.*, 2006). In addition, fluorene derivatives have found many applications in chemistry, especially in the optoelectronic area (Saragi *et al.*, 2004). In view of these important properties, the crystal structure of the title compond has been determined.

In the title compound (Fig.1), the C12—N1—C14 angle of 120.76 (15)° and the N1—C12 bond distance of 1.278 (2)Å are in close agreement with the similar *N*fluorenylideneaniline (Glagovich *et al.*, 2004; Peters *et al.*, 1998; Pierre *et al.*, 1997). The fluorene unit is essentially planar and the benzene ring bound to the imine N atom bears a methyl that is nearly coplanar. The dihedral angle between the substituent benzene ring and the 9*H*-fluoren-9-imine unit is 108.9 (3)°. Intermolecular $\pi\cdots\pi$ interactions between the benzene rings of adjacent fluorene units [centroid-centroid distance is 3.8081 (13) Å, the average perpendicular distance is 3.469 Å, the dihedral angle between the rings is 3.7°, symmetry code = -1 + *x*, *y*, *z*] are present in the crystal structure, resulting in a one-dimensional supramolecular architecture (Fig. 2).

S2. Experimental

The title compound was obtained from the condensation reaction of 9-fluorenone and 4-methylaniline as described in literature (Glagovich *et al.*, 2004) and recrystallized from ethanol solution at room temperature to give the desired product as yellow crystals suitable for single-crystal X-ray diffraction.

S3. Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with U_{iso}(H)=1.2U_{eq}(C) (1.5U_{eq} for methyl H).

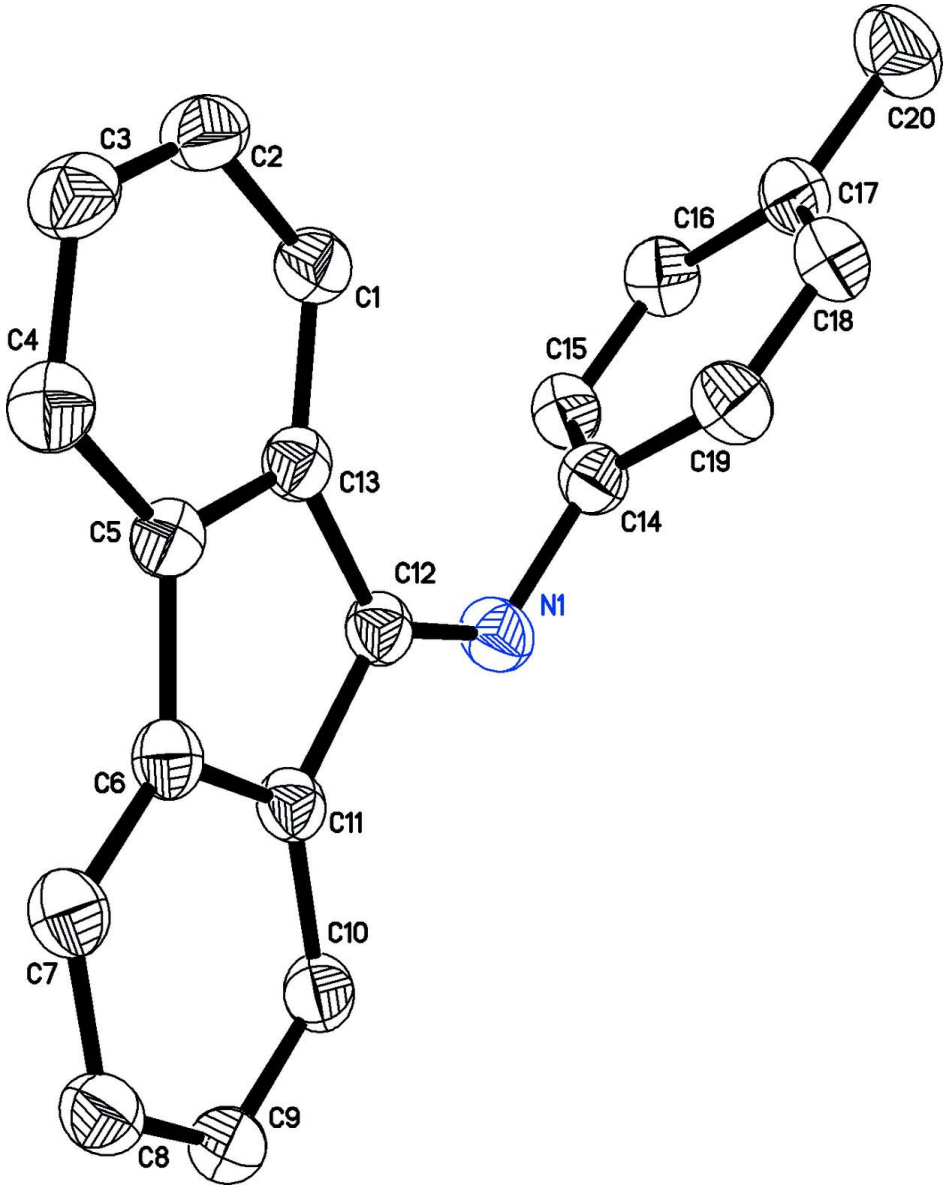

Figure 1

The molecular structure of the title compound with displacement ellipsoids at the 30% probability level. H atoms are omitted for clarity.

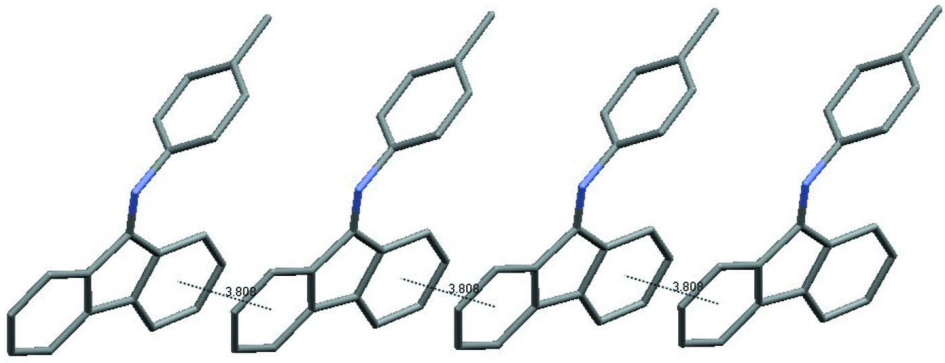

Figure 2

Partial view of the crystal packing showing the formation of the chain motif of molecules formed by the intermolecular $\pi\cdots\pi$ interactions. H atoms are omitted for clarity.

N-(9*H*-Fluoren-9-ylidene)-4-methylaniline

Crystal data

$C_{20}H_{15}N$
$M_r = 269.33$
Monoclinic, $P2_1/n$
$a = 5.6423$ (10) Å
$b = 12.187$ (2) Å
$c = 21.310$ (4) Å
$\beta = 94.441$ (2)°
$V = 1460.9$ (5) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.225$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1911 reflections
$\theta = 2.5$–22.3°
$\mu = 0.07$ mm^{-1}
$T = 294$ K
Block, yellow
0.35 × 0.17 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.976$, $T_{max} = 0.994$
10793 measured reflections
2711 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$
$h = -6\rightarrow6$
$k = -14\rightarrow14$
$l = -25\rightarrow25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.115$
$S = 1.01$
2711 reflections
192 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
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.1725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0105 (19)

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}
C1	0.0001 (3)	0.30235 (15)	0.13059 (9)	0.0507 (5)
H1	−0.0938	0.3086	0.0929	0.061*
C2	−0.0545 (4)	0.36053 (16)	0.18339 (10)	0.0582 (5)
H2	−0.1869	0.4062	0.1810	0.070*
C3	0.0836 (4)	0.35188 (16)	0.23918 (10)	0.0604 (5)
H3	0.0452	0.3931	0.2737	0.072*
C4	0.2787 (3)	0.28289 (15)	0.24478 (9)	0.0544 (5)
H4	0.3701	0.2762	0.2828	0.065*
C5	0.3348 (3)	0.22414 (13)	0.19248 (8)	0.0435 (4)
C6	0.5230 (3)	0.14217 (13)	0.18583 (8)	0.0433 (4)
C7	0.7076 (3)	0.10822 (14)	0.22712 (9)	0.0508 (5)
H7	0.7270	0.1372	0.2676	0.061*
C8	0.8643 (3)	0.03010 (15)	0.20743 (9)	0.0549 (5)
H8	0.9901	0.0065	0.2349	0.066*
C9	0.8350 (3)	−0.01288 (16)	0.14735 (9)	0.0557 (5)
H9	0.9409	−0.0657	0.1350	0.067*
C10	0.6513 (3)	0.02124 (14)	0.10530 (9)	0.0506 (5)
H10	0.6328	−0.0077	0.0648	0.061*
C11	0.4954 (3)	0.09953 (13)	0.12487 (8)	0.0432 (4)
C12	0.2980 (3)	0.15766 (13)	0.08907 (8)	0.0440 (4)
C13	0.1986 (3)	0.23442 (13)	0.13519 (8)	0.0428 (4)
C14	0.0834 (3)	0.21043 (15)	−0.00479 (8)	0.0481 (5)
C15	−0.1301 (3)	0.17101 (16)	−0.03143 (9)	0.0544 (5)
H15	−0.1735	0.0986	−0.0246	0.065*
C16	−0.2793 (4)	0.23849 (16)	−0.06821 (9)	0.0598 (5)
H16	−0.4241	0.2110	−0.0852	0.072*
C17	−0.2197 (4)	0.34635 (17)	−0.08065 (9)	0.0579 (5)
C18	−0.0037 (4)	0.38372 (16)	−0.05457 (9)	0.0612 (5)
H18	0.0417	0.4554	−0.0625	0.073*
C19	0.1475 (4)	0.31784 (16)	−0.01699 (9)	0.0592 (5)
H19	0.2921	0.3454	0.0001	0.071*

C20	−0.3829 (4)	0.4195 (2)	−0.12150 (12)	0.0880 (8)
H20A	−0.3234	0.4263	−0.1623	0.132*
H20B	−0.3899	0.4907	−0.1024	0.132*
H20C	−0.5393	0.3880	−0.1257	0.132*
N1	0.2459 (3)	0.14086 (12)	0.03045 (7)	0.0521 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0542 (11)	0.0462 (10)	0.0518 (11)	0.0015 (9)	0.0048 (9)	0.0011 (9)
C2	0.0594 (12)	0.0508 (11)	0.0659 (14)	0.0066 (9)	0.0144 (11)	−0.0045 (10)
C3	0.0717 (14)	0.0513 (12)	0.0600 (13)	0.0007 (10)	0.0164 (11)	−0.0119 (10)
C4	0.0629 (12)	0.0494 (11)	0.0507 (11)	−0.0054 (9)	0.0037 (9)	−0.0071 (9)
C5	0.0486 (10)	0.0379 (9)	0.0443 (10)	−0.0061 (8)	0.0062 (8)	−0.0038 (8)
C6	0.0477 (10)	0.0395 (9)	0.0429 (10)	−0.0065 (8)	0.0040 (8)	0.0014 (8)
C7	0.0565 (11)	0.0494 (11)	0.0457 (11)	−0.0039 (9)	−0.0005 (9)	0.0003 (9)
C8	0.0497 (11)	0.0555 (12)	0.0587 (13)	0.0015 (9)	−0.0008 (10)	0.0083 (10)
C9	0.0585 (12)	0.0521 (11)	0.0578 (13)	0.0085 (9)	0.0123 (10)	0.0071 (10)
C10	0.0630 (12)	0.0441 (10)	0.0455 (11)	0.0034 (9)	0.0102 (9)	0.0023 (8)
C11	0.0497 (10)	0.0365 (9)	0.0438 (10)	−0.0017 (8)	0.0053 (8)	0.0022 (8)
C12	0.0509 (11)	0.0381 (9)	0.0434 (11)	−0.0027 (8)	0.0064 (8)	0.0007 (8)
C13	0.0494 (10)	0.0350 (9)	0.0446 (10)	−0.0043 (8)	0.0075 (8)	−0.0004 (8)
C14	0.0591 (12)	0.0486 (10)	0.0366 (10)	0.0046 (9)	0.0029 (9)	−0.0027 (8)
C15	0.0632 (12)	0.0498 (11)	0.0502 (11)	−0.0031 (10)	0.0038 (10)	0.0021 (9)
C16	0.0562 (12)	0.0647 (13)	0.0572 (12)	−0.0059 (10)	−0.0030 (10)	0.0009 (10)
C17	0.0627 (13)	0.0626 (13)	0.0478 (11)	0.0034 (10)	0.0006 (10)	0.0082 (10)
C18	0.0700 (14)	0.0521 (12)	0.0610 (13)	−0.0019 (10)	0.0020 (11)	0.0089 (10)
C19	0.0609 (12)	0.0554 (12)	0.0597 (13)	−0.0027 (10)	−0.0046 (10)	0.0022 (10)
C20	0.0844 (17)	0.0904 (18)	0.0862 (18)	0.0081 (14)	−0.0126 (14)	0.0261 (14)
N1	0.0638 (10)	0.0489 (9)	0.0431 (9)	0.0066 (8)	0.0002 (8)	−0.0012 (7)

Geometric parameters (Å, º)

C1—C2	1.385 (3)	C10—H10	0.9300
C1—C13	1.390 (2)	C11—C12	1.481 (2)
C1—H1	0.9300	C12—N1	1.278 (2)
C2—C3	1.374 (3)	C12—C13	1.497 (2)
C2—H2	0.9300	C14—C15	1.378 (2)
C3—C4	1.383 (3)	C14—C19	1.388 (3)
C3—H3	0.9300	C14—N1	1.420 (2)
C4—C5	1.382 (2)	C15—C16	1.378 (3)
C4—H4	0.9300	C15—H15	0.9300
C5—C13	1.397 (2)	C16—C17	1.387 (3)
C5—C6	1.473 (2)	C16—H16	0.9300
C6—C7	1.374 (2)	C17—C18	1.377 (3)
C6—C11	1.397 (2)	C17—C20	1.509 (3)
C7—C8	1.386 (3)	C18—C19	1.381 (3)
C7—H7	0.9300	C18—H18	0.9300

C8—C9	1.381 (3)	C19—H19	0.9300
C8—H8	0.9300	C20—H20A	0.9600
C9—C10	1.381 (2)	C20—H20B	0.9600
C9—H9	0.9300	C20—H20C	0.9600
C10—C11	1.384 (2)		

C2—C1—C13	118.45 (18)	C6—C11—C12	109.05 (15)
C2—C1—H1	120.8	N1—C12—C11	122.27 (16)
C13—C1—H1	120.8	N1—C12—C13	132.28 (16)
C3—C2—C1	121.13 (18)	C11—C12—C13	105.42 (14)
C3—C2—H2	119.4	C1—C13—C5	120.05 (16)
C1—C2—H2	119.4	C1—C13—C12	131.81 (16)
C2—C3—C4	121.03 (18)	C5—C13—C12	108.00 (15)
C2—C3—H3	119.5	C15—C14—C19	118.94 (17)
C4—C3—H3	119.5	C15—C14—N1	121.18 (17)
C5—C4—C3	118.41 (18)	C19—C14—N1	119.68 (17)
C5—C4—H4	120.8	C16—C15—C14	120.18 (18)
C3—C4—H4	120.8	C16—C15—H15	119.9
C4—C5—C13	120.91 (17)	C14—C15—H15	119.9
C4—C5—C6	129.85 (17)	C15—C16—C17	121.85 (19)
C13—C5—C6	109.18 (15)	C15—C16—H16	119.1
C7—C6—C11	120.53 (16)	C17—C16—H16	119.1
C7—C6—C5	131.23 (16)	C18—C17—C16	117.14 (18)
C11—C6—C5	108.22 (15)	C18—C17—C20	121.3 (2)
C6—C7—C8	118.85 (18)	C16—C17—C20	121.6 (2)
C6—C7—H7	120.6	C17—C18—C19	121.97 (19)
C8—C7—H7	120.6	C17—C18—H18	119.0
C9—C8—C7	120.51 (18)	C19—C18—H18	119.0
C9—C8—H8	119.7	C18—C19—C14	119.90 (18)
C7—C8—H8	119.7	C18—C19—H19	120.1
C10—C9—C8	121.14 (18)	C14—C19—H19	120.1
C10—C9—H9	119.4	C17—C20—H20A	109.5
C8—C9—H9	119.4	C17—C20—H20B	109.5
C9—C10—C11	118.36 (17)	H20A—C20—H20B	109.5
C9—C10—H10	120.8	C17—C20—H20C	109.5
C11—C10—H10	120.8	H20A—C20—H20C	109.5
C10—C11—C6	120.60 (17)	H20B—C20—H20C	109.5
C10—C11—C12	130.17 (16)	C12—N1—C14	120.76 (15)

C13—C1—C2—C3	0.1 (3)	C2—C1—C13—C5	1.4 (3)
C1—C2—C3—C4	−1.4 (3)	C2—C1—C13—C12	176.50 (17)
C2—C3—C4—C5	1.2 (3)	C4—C5—C13—C1	−1.6 (3)
C3—C4—C5—C13	0.3 (3)	C6—C5—C13—C1	176.08 (15)
C3—C4—C5—C6	−176.88 (17)	C4—C5—C13—C12	−177.78 (15)
C4—C5—C6—C7	−6.8 (3)	C6—C5—C13—C12	−0.07 (18)
C13—C5—C6—C7	175.76 (17)	N1—C12—C13—C1	8.8 (3)
C4—C5—C6—C11	175.26 (18)	C11—C12—C13—C1	−173.40 (17)
C13—C5—C6—C11	−2.18 (18)	N1—C12—C13—C5	−175.62 (18)

C11—C6—C7—C8	−0.7 (3)	C11—C12—C13—C5	2.14 (17)
C5—C6—C7—C8	−178.41 (17)	C19—C14—C15—C16	−1.7 (3)
C6—C7—C8—C9	−0.1 (3)	N1—C14—C15—C16	−176.54 (17)
C7—C8—C9—C10	0.6 (3)	C14—C15—C16—C17	1.2 (3)
C8—C9—C10—C11	−0.3 (3)	C15—C16—C17—C18	0.0 (3)
C9—C10—C11—C6	−0.4 (3)	C15—C16—C17—C20	179.4 (2)
C9—C10—C11—C12	174.14 (17)	C16—C17—C18—C19	−0.7 (3)
C7—C6—C11—C10	1.0 (3)	C20—C17—C18—C19	179.9 (2)
C5—C6—C11—C10	179.15 (15)	C17—C18—C19—C14	0.2 (3)
C7—C6—C11—C12	−174.66 (15)	C15—C14—C19—C18	1.0 (3)
C5—C6—C11—C12	3.53 (18)	N1—C14—C19—C18	175.92 (17)
C10—C11—C12—N1	−0.5 (3)	C11—C12—N1—C14	−169.33 (16)
C6—C11—C12—N1	174.52 (16)	C13—C12—N1—C14	8.1 (3)
C10—C11—C12—C13	−178.57 (17)	C15—C14—N1—C12	−115.92 (19)
C6—C11—C12—C13	−3.52 (18)	C19—C14—N1—C12	69.2 (2)