organic papers

(Anthracen-9-ylmethyl)diethylamine at 100 K

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The molecular geometry in the title compound, $C_{19}H_{21}N$, is as expected for a compound of this kind. The molecules are interconnected to form layers by C—H···π interactions, some between edge-to-face molecules in the manner characteristic of polycyclic hydrocarbon compounds and others involving H atoms of both methyl groups of the methyldiethylamine substituent.

Comment

Interest in compounds capable of functioning as molecular devices has grown rapidly in the past fifteen years (Desilva *et al.*, 1997). A fundamental requirement of these systems is the ability to communicate information to the user by some appropriate means. Photo-induced electron transfer or PET-based systems, which use fluorescence emission as a method to transmit relevant data, have been employed in a variety of circumstances. Indeed, PET molecules capable of indicating the presence of cations, anions and neutral molecules have been reported (Desilva *et al.*, 1993). The mechanism by which this particular family of sensor molecules functions hinges on a 'box' or modular logic approach (Bissell *et al.*, 1993). We have previously reported the structure of a PET fluorescent saccharide sensor (Barkhuizen *et al.*, 2004) based on a molecule originally synthesized by Shinkai and his group (James *et al.*, 1995). The title compound, (I), presented here is representative of a subgroup of molecules designed to operate as single molecule pH PET sensors based on the same modular logic approach. Compound (I) alters its fluorescence emission intensity as a function of the pH of its environment in aqueous methanol solutions (Desilva & Rupasinghe, 1985).

(I)
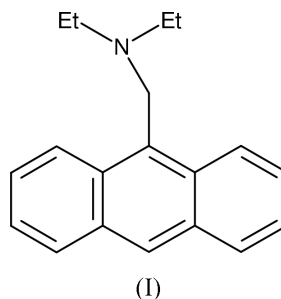
The molecule of (I) is shown in Fig. 1. Selected bond lengths and angles, primarily for the methyldiethylamine substituent, are given in Table 1. These, along with C—C distances and internal angles in the anthracene fragment in the ranges, respectively, of 1.3588 (14)–1.4451 (13) Å and 116.86 (8)–121.39 (9)°, are as expected for this type of molecule. The anthracene moiety is essentially planar with an r.m.s. dis-
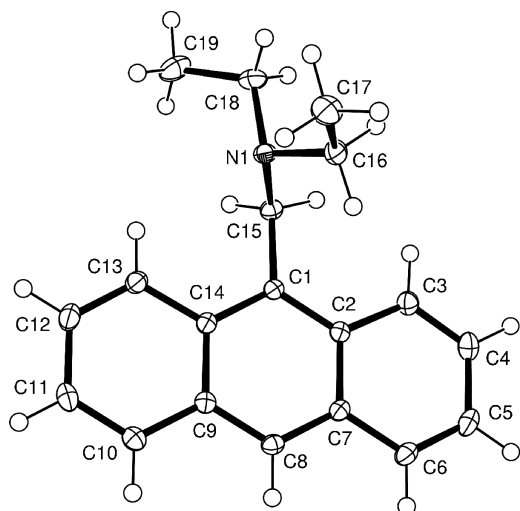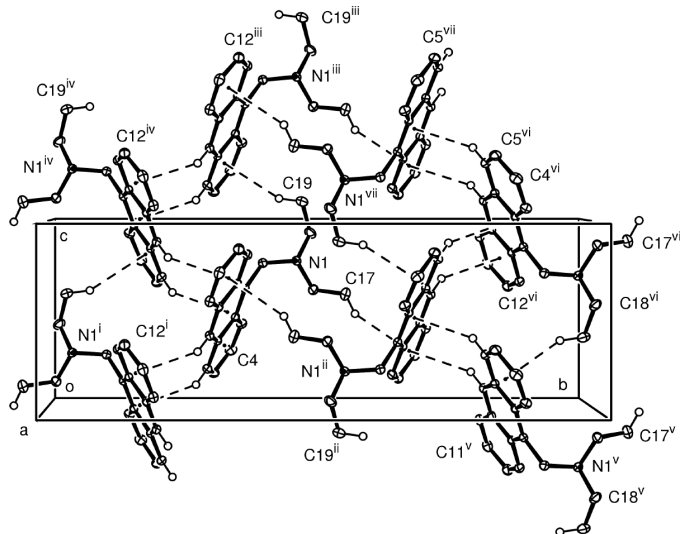
Figure 1
The molecule of (I). Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii.

Figure 2
The packing of (I). Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii. Dashed lines represent C—H···π contacts. Selected atoms are labelled. [Symmetry codes: (i) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $x, y, 1 + z$; (iv) $x, \frac{1}{2} - y, z + \frac{1}{2}$; (v) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (vi) $1 - x, \frac{1}{2} - y, \frac{3}{2} - z$; (vii) $1 - x, 1 - y, 2 - z$.]

placement for the atoms (C1–C14) which define it of 0.0234 Å. The largest displacement is that of C4 at 0.0380 (8) Å, followed by that of C7 at 0.0355 (8) Å. The displacements from the anthracene least-squares plane of atoms C15, N1, C16, C17, C18 and C19 are −0.0534 (12), 1.2190 (13), 2.2643 (15), 3.6724 (17), 1.0212 (17) and 0.2988 (18) Å, respectively. That is, as expected, atom C15 is more or less in the plane of the ring system and N1 displaced from it. The atoms of the ethyl group defined by C16–C17 are still further displaced, in the same sense as N1, while the ethyl group defined by C18–C19 is directed back towards the plane of the ring system. The torsion angles around the C15—N1 bond given in Table 1 are entirely consistent with this interpretation. The intermolecular C—H···π contacts given in Table 2 and

shown in Fig. 2 interconnect the molecules to form layers parallel to (100). The layers are related to one another purely by cell translation in the direction of a.

Experimental

Crystal data

C$_{19}$H$_{21}$N	$D_x = 1.167$ Mg m^{-3}
$M_r = 263.37$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2017
$a = 8.523$ (1) Å	reflections
$b = 22.678$ (5) Å	$\theta = 4$–32°
$c = 7.769$ (2) Å	$\mu = 0.07$ mm^{-1}
$\beta = 93.388$ (15)°	$T = 100$ (2) K
$V = 1499.0$ (5) Å^3	Cut prism, colorless
$Z = 4$	$0.30 \times 0.20 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur2 area-detector diffractometer	3585 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.024$
ω–2θ scans	$\theta_{max} = 31.9°$
Absorption correction: none	$h = -12 \rightarrow 12$
14548 measured reflections	$k = -33 \rightarrow 31$
4796 independent reflections	$l = -11 \rightarrow 8$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$
$wR(F^2) = 0.137$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
4796 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
183 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C15	1.4738 (12)	C1—C15	1.5201 (13)
N1—C16	1.4753 (13)	C16—C17	1.5183 (15)
N1—C18	1.4782 (12)	C18—C19	1.5215 (15)
C15—N1—C16	110.27 (7)	C2—C1—C15	121.86 (8)
C15—N1—C18	109.24 (8)	N1—C15—C1	113.06 (7)
C16—N1—C18	110.22 (8)	N1—C16—C17	113.32 (8)
C14—C1—C15	118.57 (8)	N1—C18—C19	113.92 (9)
C2—C1—C15—N1	−107.99 (9)	C1—C15—N1—C18	−172.35 (8)
C14—C1—C15—N1	73.42 (10)	C15—N1—C16—C17	−162.17 (8)
C1—C15—N1—C16	66.38 (10)	C15—N1—C18—C19	76.45 (11)

Table 2
Geometry (Å, °) of C—H···π contacts in (I).

C—H···Cg^a	C—H	H···Cg	$H_{perp}{}^b$	γ^c	C—H···Cg	C···Cg
C6—H6···$Cg1^i$	0.95	2.58	2.56	7	145.56	3.405
C8—H8···$Cg3^i$	0.95	2.77	2.74	9	145.74	3.595
C17—H17B···$Cg3^{ii}$	0.95	2.78	2.76	8	138.84	3.581
C19—H19A···$Cg2^{iii}$	0.95	2.91	2.89	6	150.72	3.795

Notes: (a) $Cg(n)$, n = 1 to 3, are the centroids of rings defined by C1–C2/C7–C9/C14, C2–C7 and C9–C14, respectively; (b) H_{perp} is the perpendicular distance of the H atom from the mean plane of the ring; (c) γ is the angle at hydrogen between H···Cg and H_{perp}. Symmetry codes: (i) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $x, y, 1 + z$.

In the final stages of refinement, H atoms were introduced in calculated positions, with C—H distances of 0.95, 0.99 and 0.98 Å for aryl, methylene and methyl H atoms, respectively, and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $U_{iso}(H) = 1.2U_{eq}(C)$ otherwise. The orientation of the rigid body methyl groups was also refined.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

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supporting information

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$C_{19}H_{21}N$	$F(000) = 568$
$M_r = 263.37$	$D_x = 1.167$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 360–361 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.523$ (1) Å	Cell parameters from 2017 reflections
$b = 22.678$ (5) Å	$\theta = 4$–32°
$c = 7.769$ (2) Å	$\mu = 0.07$ mm^{-1}
$\beta = 93.388$ (15)°	$T = 100$ K
$V = 1499.0$ (5) Å^3	Prism, colorless
$Z = 4$	$0.30 \times 0.20 \times 0.20$ mm

Data collection

Xcalibur2 area-detector diffractometer	3585 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.024$
Graphite monochromator	$\theta_{max} = 31.9°$, $\theta_{min} = 4.3°$
ω–2θ scans	$h = -12\rightarrow12$
14548 measured reflections	$k = -33\rightarrow31$
4796 independent reflections	$l = -11\rightarrow8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.137$	
$S = 1.06$	H-atom parameters constrained
4796 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
183 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.38$ 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.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

2.5356 (0.0016) x + 19.2959 (0.0059) y - 3.4950 (0.0017) z = 5.6313 (0.0020)

* 0.0018 (0.0008) C1 * 0.0159 (0.0008) C2 * -0.0057 (0.0008) C3 * -0.0380 (0.0008) C4 * -0.0286 (0.0008) C5 * 0.0236 (0.0008) C6 * 0.0355 (0.0008) C7 * 0.0290 (0.0008) C8 * 0.0043 (0.0008) C9 * -0.0306 (0.0008) C10 * -0.0334 (0.0008) C11 * 0.0004 (0.0008) C12 * 0.0166 (0.0008) C13 * 0.0091 (0.0008) C14 - 0.0534 (0.0012) C15 2.2643 (0.0015) C16 3.6724 (0.0017) C17 1.0212 (0.0017) C18 0.2988 (0.0018) C19 1.2190 (0.0013) N1

Rms deviation of fitted atoms = 0.0234

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}
N1	0.28466 (10)	0.45869 (4)	0.77896 (10)	0.01573 (18)
C1	0.32807 (10)	0.36296 (4)	0.63016 (11)	0.01304 (18)
C2	0.25325 (11)	0.34470 (4)	0.47101 (11)	0.01319 (18)
C3	0.09093 (11)	0.35617 (4)	0.42278 (12)	0.0178 (2)
H3	0.0298	0.3783	0.4982	0.021*
C4	0.02237 (12)	0.33592 (5)	0.27049 (13)	0.0214 (2)
H4	−0.0858	0.3437	0.2431	0.026*
C5	0.11017 (12)	0.30347 (5)	0.15230 (13)	0.0209 (2)
H5	0.0606	0.2894	0.0475	0.025*
C6	0.26519 (12)	0.29265 (4)	0.19013 (12)	0.0177 (2)
H6	0.3240	0.2718	0.1096	0.021*
C7	0.34132 (11)	0.31209 (4)	0.34929 (11)	0.01392 (18)
C8	0.49882 (11)	0.29836 (4)	0.38961 (12)	0.01495 (19)
H8	0.5561	0.2769	0.3091	0.018*
C9	0.57381 (10)	0.31564 (4)	0.54650 (11)	0.01381 (18)
C10	0.73430 (11)	0.30030 (4)	0.58820 (12)	0.0170 (2)
H10	0.7900	0.2776	0.5092	0.020*
C11	0.80842 (11)	0.31788 (4)	0.73983 (13)	0.0195 (2)
H11	0.9150	0.3073	0.7660	0.023*
C12	0.72597 (12)	0.35206 (4)	0.85905 (13)	0.0206 (2)
H12	0.7789	0.3647	0.9637	0.025*
C13	0.57198 (11)	0.36699 (4)	0.82513 (12)	0.0176 (2)
H13	0.5193	0.3896	0.9070	0.021*
C14	0.48826 (11)	0.34909 (4)	0.66770 (11)	0.01342 (18)
C15	0.23994 (11)	0.39603 (4)	0.76462 (12)	0.01584 (19)
H15A	0.1257	0.3933	0.7344	0.019*
H15B	0.2607	0.3768	0.8781	0.019*
C16	0.23523 (12)	0.49040 (4)	0.61903 (13)	0.0197 (2)
H16A	0.1205	0.4975	0.6171	0.024*

H16B	0.2560	0.4651	0.5190	0.024*
C17	0.31859 (14)	0.54901 (5)	0.60020 (14)	0.0264 (2)
H17A	0.2947	0.5750	0.6961	0.040*
H17B	0.2826	0.5675	0.4909	0.040*
H17C	0.4323	0.5424	0.6015	0.040*
C18	0.21012 (12)	0.48517 (5)	0.92764 (13)	0.0233 (2)
H18A	0.0989	0.4725	0.9252	0.028*
H18B	0.2113	0.5286	0.9154	0.028*
C19	0.28961 (15)	0.46879 (5)	1.10158 (13)	0.0280 (3)
H19A	0.2835	0.4260	1.1181	0.042*
H19B	0.2365	0.4888	1.1935	0.042*
H19C	0.4001	0.4810	1.1052	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0197 (4)	0.0139 (4)	0.0136 (4)	0.0019 (3)	0.0014 (3)	−0.0014 (3)
C1	0.0153 (4)	0.0115 (4)	0.0124 (4)	−0.0006 (3)	0.0009 (3)	0.0011 (3)
C2	0.0147 (4)	0.0112 (4)	0.0136 (4)	−0.0010 (3)	0.0005 (3)	0.0017 (3)
C3	0.0168 (5)	0.0199 (5)	0.0167 (4)	0.0004 (3)	0.0006 (3)	0.0016 (3)
C4	0.0166 (5)	0.0262 (5)	0.0208 (5)	−0.0013 (4)	−0.0032 (4)	0.0033 (4)
C5	0.0253 (5)	0.0217 (5)	0.0150 (4)	−0.0042 (4)	−0.0050 (4)	−0.0004 (4)
C6	0.0237 (5)	0.0150 (4)	0.0141 (4)	−0.0018 (3)	−0.0007 (4)	−0.0013 (3)
C7	0.0175 (4)	0.0116 (4)	0.0126 (4)	−0.0016 (3)	0.0000 (3)	0.0004 (3)
C8	0.0178 (4)	0.0126 (4)	0.0145 (4)	0.0000 (3)	0.0021 (3)	−0.0007 (3)
C9	0.0150 (4)	0.0114 (4)	0.0150 (4)	−0.0012 (3)	0.0005 (3)	0.0014 (3)
C10	0.0160 (4)	0.0151 (4)	0.0200 (5)	0.0000 (3)	0.0016 (3)	0.0014 (3)
C11	0.0149 (4)	0.0183 (5)	0.0249 (5)	−0.0003 (3)	−0.0034 (4)	0.0035 (4)
C12	0.0234 (5)	0.0186 (5)	0.0188 (5)	−0.0008 (4)	−0.0067 (4)	0.0002 (4)
C13	0.0221 (5)	0.0151 (4)	0.0154 (4)	0.0012 (3)	−0.0019 (4)	−0.0010 (3)
C14	0.0160 (4)	0.0107 (4)	0.0134 (4)	−0.0010 (3)	−0.0005 (3)	0.0013 (3)
C15	0.0182 (4)	0.0148 (4)	0.0147 (4)	−0.0007 (3)	0.0021 (3)	−0.0002 (3)
C16	0.0239 (5)	0.0166 (5)	0.0182 (5)	0.0020 (4)	−0.0028 (4)	0.0014 (4)
C17	0.0341 (6)	0.0174 (5)	0.0275 (6)	0.0000 (4)	0.0009 (5)	0.0038 (4)
C18	0.0268 (5)	0.0231 (5)	0.0206 (5)	0.0046 (4)	0.0051 (4)	−0.0064 (4)
C19	0.0420 (7)	0.0260 (6)	0.0163 (5)	−0.0029 (5)	0.0045 (4)	−0.0038 (4)

Geometric parameters (Å, º)

N1—C15	1.4738 (12)	C10—H10	0.9500
N1—C16	1.4753 (13)	C11—C12	1.4246 (15)
N1—C18	1.4782 (12)	C11—H11	0.9500
C1—C14	1.4146 (13)	C12—C13	1.3659 (14)
C1—C2	1.4191 (12)	C12—H12	0.9500
C1—C15	1.5201 (13)	C13—C14	1.4376 (13)
C2—C3	1.4355 (13)	C13—H13	0.9500
C2—C7	1.4451 (13)	C15—H15A	0.9900
C3—C4	1.3677 (14)	C15—H15B	0.9900

C3—H3	0.9500	C16—C17	1.5183 (15)
C4—C5	1.4234 (15)	C16—H16A	0.9900
C4—H4	0.9500	C16—H16B	0.9900
C5—C6	1.3588 (14)	C17—H17A	0.9800
C5—H5	0.9500	C17—H17B	0.9800
C6—C7	1.4316 (13)	C17—H17C	0.9800
C6—H6	0.9500	C18—C19	1.5215 (15)
C7—C8	1.3954 (13)	C18—H18A	0.9900
C8—C9	1.3984 (13)	C18—H18B	0.9900
C8—H8	0.9500	C19—H19A	0.9800
C9—C10	1.4299 (13)	C19—H19B	0.9800
C9—C14	1.4403 (13)	C19—H19C	0.9800
C10—C11	1.3630 (13)		
C15—N1—C16	110.27 (7)	C11—C12—H12	119.5
C15—N1—C18	109.24 (8)	C12—C13—C14	121.14 (9)
C16—N1—C18	110.22 (8)	C12—C13—H13	119.4
C14—C1—C2	119.56 (8)	C14—C13—H13	119.4
C14—C1—C15	118.57 (8)	C1—C14—C13	122.49 (8)
C2—C1—C15	121.86 (8)	C1—C14—C9	120.13 (8)
C1—C2—C3	123.44 (8)	C13—C14—C9	117.38 (8)
C1—C2—C7	119.70 (8)	N1—C15—C1	113.06 (7)
C3—C2—C7	116.86 (8)	N1—C15—H15A	109.0
C4—C3—C2	121.39 (9)	C1—C15—H15A	109.0
C4—C3—H3	119.3	N1—C15—H15B	109.0
C2—C3—H3	119.3	C1—C15—H15B	109.0
C3—C4—C5	121.17 (9)	H15A—C15—H15B	107.8
C3—C4—H4	119.4	N1—C16—C17	113.32 (8)
C5—C4—H4	119.4	N1—C16—H16A	108.9
C6—C5—C4	119.69 (9)	C17—C16—H16A	108.9
C6—C5—H5	120.2	N1—C16—H16B	108.9
C4—C5—H5	120.2	C17—C16—H16B	108.9
C5—C6—C7	121.10 (9)	H16A—C16—H16B	107.7
C5—C6—H6	119.4	C16—C17—H17A	109.5
C7—C6—H6	119.4	C16—C17—H17B	109.5
C8—C7—C6	120.41 (8)	H17A—C17—H17B	109.5
C8—C7—C2	119.82 (8)	C16—C17—H17C	109.5
C6—C7—C2	119.75 (8)	H17A—C17—H17C	109.5
C7—C8—C9	121.15 (8)	H17B—C17—H17C	109.5
C7—C8—H8	119.4	N1—C18—C19	113.92 (9)
C9—C8—H8	119.4	N1—C18—H18A	108.8
C8—C9—C10	120.74 (8)	C19—C18—H18A	108.8
C8—C9—C14	119.63 (8)	N1—C18—H18B	108.8
C10—C9—C14	119.63 (8)	C19—C18—H18B	108.8
C11—C10—C9	120.86 (9)	H18A—C18—H18B	107.7
C11—C10—H10	119.6	C18—C19—H19A	109.5
C9—C10—H10	119.6	C18—C19—H19B	109.5
C10—C11—C12	119.99 (9)	H19A—C19—H19B	109.5

C10—C11—H11	120.0	C18—C19—H19C	109.5
C12—C11—H11	120.0	H19A—C19—H19C	109.5
C13—C12—C11	120.98 (9)	H19B—C19—H19C	109.5
C13—C12—H12	119.5		
C2—C1—C15—N1	−107.99 (9)	C1—C15—N1—C18	−172.35 (8)
C14—C1—C15—N1	73.42 (10)	C15—N1—C16—C17	−162.17 (8)
C1—C15—N1—C16	66.38 (10)	C15—N1—C18—C19	76.45 (11)