Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Ethoxy-2-methoxy-4-[2-(4-nitrophenyl)ethenyl]benzene

Paul M. Dinakaran,[a] S. Kalainathan,[a]* T. Srinivasan[b] and D. Velmurugan[b]

[a]Crystal Research Centre, School of Advanced Sciences, VIT University, Vellore 632 014, Tamil Nadu, India, and [b]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: Kalainathan@yahoo.com

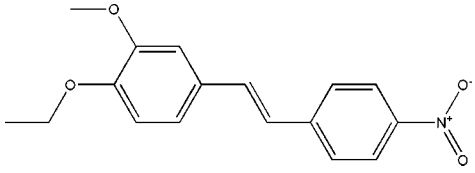
Received 25 July 2012; accepted 1 August 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.138; data-to-parameter ratio = 18.8.

In the title molecule, $C_{17}H_{17}NO_4$, the dihedral angle between the two aromatic rings is 42.47 (7)°. The nitro group is twisted by 7.44 (11)° out of the plane of the ring to which it is attached. The methoxy and ethoxy group O atoms deviate significantly from the phenyl ring [by 0.0108 (11) and 0.0449 (11) Å, respectively]. The crystal structure is stabilized by C—H···π interactions.

Related literature

For the synthesis of the title compound, see: Tam *et al.* (1989). For hybridization, see: Beddoes *et al.* (1986)



Experimental

Crystal data

$C_{17}H_{17}NO_4$
M_r = 299.32
Monoclinic, $P2_1/n$
a = 8.5209 (4) Å
b = 7.5959 (4) Å
c = 23.7877 (13) Å
β = 99.611 (3)°
V = 1518.02 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
14265 measured reflections
3789 independent reflections
2831 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.138
S = 1.04
3789 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C9–C14 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17A···*Cg*2	0.97	2.96	3.281 (2)	145

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

TS and DV thank the TBI X-ray facility, CAS in Crystallography and Biophysics, University of Madras, India, for data collection and TS thanks DST for the Inspire fellowship. PMD and SK thank SERC–DST for providing financial support and VIT University management for their constant encouragement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5986).

References

Beddoes, R. L., Dalton, L., Joule, T. A., Mills, O. S. , Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans.* **2**, pp. 787–797.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tam, W., Guerin, B., Calabrese, J. C. & Stevenson, H. S. (1989). *Chem. Phys. Lett.* **154**, 93–96.

supplementary materials

Acta Cryst. (2012). E**68**, o2774 [doi:10.1107/S1600536812034320]

1-Ethoxy-2-methoxy-4-[2-(4-nitrophenyl)ethenyl]benzene

Paul M. Dinakaran, S. Kalainathan, T. Srinivasan and D. Velmurugan

Comment

The dihedral angle between nitro substituted phenyl ring (C1-C6) & oxygen substituted benzene ring (C9-C14) is 42.47 (7)°. The sum of bond angles around N1 (359.59°) is in accordance with sp_2 hybridization (Beddoes *et al.*, 1986). The methoxy and ethoxy group O3 and O4 atoms are significantly deviated from the phenyl ring (C9–C13) with the values of -0.0108 (11) Å and -0.0449 (11) Å, respectively.

A weak intermolecular C—H···π interaction involving the C17–H17A group and the C9–C14 benzene ring (centroid Cg2) of the molecule at (2-x,-y,-z) is observed [H17A···Cg2 = 2.96 Å, C17···Cg2 = 3.781 (2) Å and C17-H17A···Cg2 = 145°].

Experimental

4-Ethoxy 3-Methoxy 4-Nitrostilbene (4E3MONS) is a derivative material of stilebene.The material (4E3MONS) was synthesized by Witting reaction method. The material was prepared from the 4-ethoxy 3-methoxy benzaldehyde and di-ethyl p-nitrobenzyl phosphonate in the presence of sodium ethoxide catalyst. The steps involved during the chemical reactions are as follows: the calculated amount of diethyl p-nitrobenzyl phosphonate (0.01 mol %, 2.2304ml) and 4-eth-oxy 3-methoxy benzaldehyde (0.01 mol, 1.802 ml %) were added in the ethanol solution (35 ml). After the reaction process, the sodium ethoxide,which plays a role of catalyst, was added immediately the colour of the solution became red. Then the mixture was stirred for 12 hrs at ice cold temperature in ultracryostat which has stirrer rotation facility. After the stirring process completed, the orange colour 4E3MONS material was collected from the mixture by removing the ethanol (Tam *et al.*, 1989). Then the 4E3MONS was purified by a successive recrystallization process.

Refinement

Hydrogen atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding model with fixed isotropic displacement parameter: U_{iso}(H) = 1.2 U_{eq}(C).

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

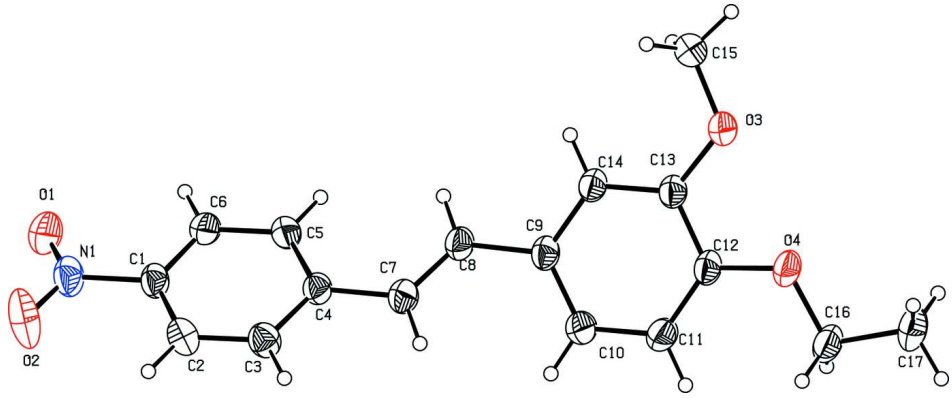


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

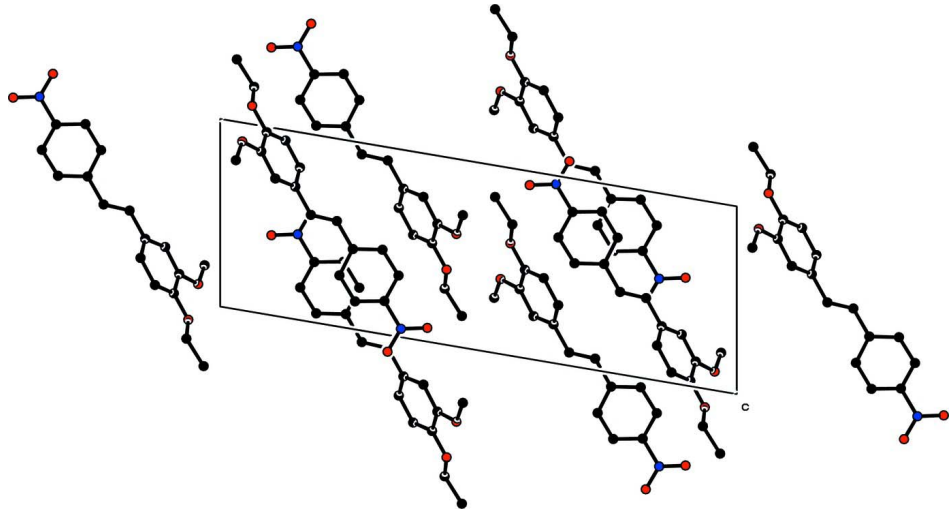


Figure 2

A view of the C—H···N and C—H···O hydrogen bonds (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) - *x* + 1, - *y* -1, - *z*; (ii) - *x* +1/2, *y* - 1/2, - *z* + 1/2.]

1-Ethoxy-2-methoxy-4-[2-(4-nitrophenyl)ethenyl]benzene

Crystal data

$C_{17}H_{17}NO_4$
M_r = 299.32
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.5209 (4) Å
b = 7.5959 (4) Å
c = 23.7877 (13) Å
β = 99.611 (3)°
V = 1518.02 (14) Å^3
Z = 4

$F(000)$ = 632
D_x = 1.310 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3789 reflections
θ = 1.7–28.5°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
14265 measured reflections
3789 independent reflections
2831 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.5°$, $\theta_{min} = 1.7°$
$h = -11 \rightarrow 11$
$k = -9 \rightarrow 9$
$l = -31 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.138$
$S = 1.04$
3789 reflections
202 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
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.2742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.121 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O4	1.09886 (11)	0.13016 (14)	0.06184 (5)	0.0622 (3)
O3	0.89997 (12)	0.38803 (13)	0.04273 (5)	0.0619 (3)
C9	0.70663 (15)	0.13692 (18)	0.14525 (6)	0.0488 (3)
C13	0.86351 (14)	0.26322 (17)	0.07949 (5)	0.0468 (3)
C4	0.42645 (15)	0.09455 (17)	0.25675 (6)	0.0469 (3)
N1	0.04474 (16)	0.11093 (17)	0.34984 (6)	0.0644 (4)
C1	0.17789 (16)	0.10582 (17)	0.31788 (6)	0.0508 (3)
C8	0.57030 (15)	0.15205 (19)	0.17555 (6)	0.0512 (3)
H8	0.4829	0.2161	0.1578	0.061*
C14	0.73211 (14)	0.26748 (18)	0.10663 (5)	0.0478 (3)
H14	0.6594	0.3592	0.0990	0.057*
C6	0.14936 (16)	0.14921 (19)	0.26099 (6)	0.0545 (3)
H6	0.0478	0.1812	0.2432	0.065*
C10	0.81278 (17)	−0.0027 (2)	0.15429 (7)	0.0584 (4)
H10	0.7962	−0.0925	0.1792	0.070*
C5	0.27400 (16)	0.14451 (19)	0.23074 (6)	0.0529 (3)

H5	0.2561	0.1752	0.1924	0.063*
C12	0.97140 (15)	0.12289 (18)	0.08991 (6)	0.0496 (3)
C11	0.94367 (16)	−0.0096 (2)	0.12641 (7)	0.0583 (4)
H11	1.0131	−0.1048	0.1325	0.070*
C7	0.56122 (15)	0.08254 (19)	0.22582 (6)	0.0538 (3)
H7	0.6494	0.0195	0.2434	0.065*
O1	−0.08925 (15)	0.13496 (19)	0.32390 (7)	0.0886 (4)
C3	0.44945 (16)	0.0507 (2)	0.31410 (6)	0.0556 (3)
H3	0.5502	0.0165	0.3321	0.067*
C16	1.20153 (17)	−0.0197 (2)	0.06557 (7)	0.0630 (4)
H16A	1.1425	−0.1227	0.0499	0.076*
H16B	1.2462	−0.0435	0.1051	0.076*
C2	0.32634 (17)	0.0564 (2)	0.34522 (6)	0.0579 (4)
H2	0.3435	0.0274	0.3837	0.070*
C17	1.33198 (18)	0.0214 (3)	0.03219 (8)	0.0733 (5)
H17A	1.2867	0.0416	−0.0070	0.110*
H17B	1.4046	−0.0759	0.0347	0.110*
H17C	1.3880	0.1250	0.0476	0.110*
C15	0.7940 (2)	0.5327 (2)	0.03028 (7)	0.0693 (4)
H15A	0.6912	0.4905	0.0128	0.104*
H15B	0.8345	0.6119	0.0047	0.104*
H15C	0.7848	0.5935	0.0650	0.104*
O2	0.07343 (17)	0.0848 (2)	0.40088 (6)	0.1057 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0506 (5)	0.0632 (6)	0.0811 (7)	0.0073 (4)	0.0349 (5)	0.0034 (5)
O3	0.0615 (6)	0.0597 (6)	0.0727 (7)	0.0083 (5)	0.0347 (5)	0.0121 (5)
C9	0.0411 (6)	0.0529 (7)	0.0553 (7)	−0.0035 (5)	0.0169 (5)	−0.0032 (6)
C13	0.0448 (6)	0.0474 (7)	0.0511 (7)	−0.0029 (5)	0.0167 (5)	−0.0033 (5)
C4	0.0443 (6)	0.0456 (7)	0.0534 (7)	−0.0031 (5)	0.0155 (5)	0.0005 (5)
N1	0.0640 (8)	0.0611 (8)	0.0759 (9)	−0.0142 (6)	0.0349 (7)	−0.0055 (6)
C1	0.0525 (7)	0.0461 (7)	0.0592 (8)	−0.0081 (5)	0.0247 (6)	−0.0038 (6)
C8	0.0429 (6)	0.0531 (7)	0.0611 (8)	0.0003 (5)	0.0190 (6)	0.0011 (6)
C14	0.0426 (6)	0.0496 (7)	0.0540 (7)	0.0011 (5)	0.0159 (5)	−0.0040 (6)
C6	0.0465 (7)	0.0549 (8)	0.0647 (9)	0.0044 (6)	0.0169 (6)	0.0081 (6)
C10	0.0531 (7)	0.0541 (8)	0.0730 (10)	0.0013 (6)	0.0252 (7)	0.0095 (7)
C5	0.0496 (7)	0.0595 (8)	0.0522 (7)	0.0033 (6)	0.0157 (6)	0.0090 (6)
C12	0.0411 (6)	0.0530 (7)	0.0586 (8)	−0.0017 (5)	0.0195 (5)	−0.0055 (6)
C11	0.0496 (7)	0.0528 (8)	0.0770 (10)	0.0071 (6)	0.0234 (7)	0.0046 (7)
C7	0.0420 (6)	0.0619 (8)	0.0594 (8)	0.0016 (6)	0.0145 (6)	0.0035 (7)
O1	0.0603 (7)	0.1011 (10)	0.1138 (10)	0.0131 (7)	0.0422 (7)	0.0163 (8)
C3	0.0479 (7)	0.0656 (9)	0.0531 (8)	−0.0037 (6)	0.0082 (6)	0.0046 (7)
C16	0.0515 (7)	0.0690 (10)	0.0734 (10)	0.0109 (7)	0.0250 (7)	−0.0059 (8)
C2	0.0604 (8)	0.0668 (9)	0.0485 (7)	−0.0102 (7)	0.0143 (6)	0.0016 (6)
C17	0.0513 (8)	0.0977 (13)	0.0768 (11)	0.0075 (8)	0.0276 (7)	−0.0102 (9)
C15	0.0742 (10)	0.0692 (10)	0.0708 (10)	0.0166 (8)	0.0301 (8)	0.0191 (8)
O2	0.0873 (9)	0.1721 (16)	0.0668 (8)	−0.0343 (10)	0.0395 (7)	−0.0100 (9)

Geometric parameters (Å, º)

O4—C12	1.3678 (14)	C6—C5	1.3791 (18)
O4—C16	1.4296 (17)	C6—H6	0.9300
O3—C13	1.3605 (16)	C10—C11	1.3905 (18)
O3—C15	1.4218 (18)	C10—H10	0.9300
C9—C10	1.3871 (19)	C5—H5	0.9300
C9—C14	1.3933 (19)	C12—C11	1.375 (2)
C9—C8	1.4702 (17)	C11—H11	0.9300
C13—C14	1.3831 (16)	C7—H7	0.9300
C13—C12	1.4024 (18)	C3—C2	1.3818 (19)
C4—C3	1.386 (2)	C3—H3	0.9300
C4—C5	1.3950 (18)	C16—C17	1.503 (2)
C4—C7	1.4664 (18)	C16—H16A	0.9700
N1—O2	1.2141 (19)	C16—H16B	0.9700
N1—O1	1.2175 (19)	C2—H2	0.9300
N1—C1	1.4678 (17)	C17—H17A	0.9600
C1—C2	1.375 (2)	C17—H17B	0.9600
C1—C6	1.375 (2)	C17—H17C	0.9600
C8—C7	1.321 (2)	C15—H15A	0.9600
C8—H8	0.9300	C15—H15B	0.9600
C14—H14	0.9300	C15—H15C	0.9600
C12—O4—C16	117.72 (11)	O4—C12—C13	115.69 (12)
C13—O3—C15	117.87 (10)	C11—C12—C13	119.43 (11)
C10—C9—C14	118.49 (12)	C12—C11—C10	120.62 (13)
C10—C9—C8	122.14 (12)	C12—C11—H11	119.7
C14—C9—C8	119.37 (12)	C10—C11—H11	119.7
O3—C13—C14	124.98 (12)	C8—C7—C4	126.75 (13)
O3—C13—C12	115.47 (11)	C8—C7—H7	116.6
C14—C13—C12	119.54 (12)	C4—C7—H7	116.6
C3—C4—C5	118.04 (12)	C2—C3—C4	121.63 (13)
C3—C4—C7	119.01 (12)	C2—C3—H3	119.2
C5—C4—C7	122.94 (12)	C4—C3—H3	119.2
O2—N1—O1	123.13 (14)	O4—C16—C17	107.48 (14)
O2—N1—C1	118.00 (14)	O4—C16—H16A	110.2
O1—N1—C1	118.82 (14)	C17—C16—H16A	110.2
C2—C1—C6	121.92 (12)	O4—C16—H16B	110.2
C2—C1—N1	119.48 (13)	C17—C16—H16B	110.2
C6—C1—N1	118.59 (13)	H16A—C16—H16B	108.5
C7—C8—C9	125.65 (13)	C1—C2—C3	118.44 (13)
C7—C8—H8	117.2	C1—C2—H2	120.8
C9—C8—H8	117.2	C3—C2—H2	120.8
C13—C14—C9	121.24 (12)	C16—C17—H17A	109.5
C13—C14—H14	119.4	C16—C17—H17B	109.5
C9—C14—H14	119.4	H17A—C17—H17B	109.5
C1—C6—C5	118.84 (13)	C16—C17—H17C	109.5
C1—C6—H6	120.6	H17A—C17—H17C	109.5
C5—C6—H6	120.6	H17B—C17—H17C	109.5
C9—C10—C11	120.61 (13)	O3—C15—H15A	109.5

C9—C10—H10	119.7	O3—C15—H15B	109.5
C11—C10—H10	119.7	H15A—C15—H15B	109.5
C6—C5—C4	121.13 (13)	O3—C15—H15C	109.5
C6—C5—H5	119.4	H15A—C15—H15C	109.5
C4—C5—H5	119.4	H15B—C15—H15C	109.5
O4—C12—C11	124.88 (12)		

C15—O3—C13—C14	−1.2 (2)	C16—O4—C12—C11	7.3 (2)
C15—O3—C13—C12	179.55 (13)	C16—O4—C12—C13	−172.56 (13)
O2—N1—C1—C2	5.9 (2)	O3—C13—C12—O4	0.07 (18)
O1—N1—C1—C2	−171.61 (15)	C14—C13—C12—O4	−179.27 (12)
O2—N1—C1—C6	−174.80 (15)	O3—C13—C12—C11	−179.80 (13)
O1—N1—C1—C6	7.7 (2)	C14—C13—C12—C11	0.9 (2)
C10—C9—C8—C7	25.6 (2)	O4—C12—C11—C10	178.12 (14)
C14—C9—C8—C7	−153.64 (15)	C13—C12—C11—C10	−2.0 (2)
O3—C13—C14—C9	−177.74 (13)	C9—C10—C11—C12	0.8 (2)
C12—C13—C14—C9	1.5 (2)	C9—C8—C7—C4	−179.53 (13)
C10—C9—C14—C13	−2.7 (2)	C3—C4—C7—C8	−164.96 (15)
C8—C9—C14—C13	176.55 (12)	C5—C4—C7—C8	16.6 (2)
C2—C1—C6—C5	−0.7 (2)	C5—C4—C3—C2	−0.3 (2)
N1—C1—C6—C5	−179.95 (13)	C7—C4—C3—C2	−178.83 (13)
C14—C9—C10—C11	1.5 (2)	C12—O4—C16—C17	−179.27 (13)
C8—C9—C10—C11	−177.69 (14)	C6—C1—C2—C3	0.0 (2)
C1—C6—C5—C4	0.9 (2)	N1—C1—C2—C3	179.29 (13)
C3—C4—C5—C6	−0.4 (2)	C4—C3—C2—C1	0.5 (2)
C7—C4—C5—C6	178.09 (13)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C9–C14 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*A*···*Cg*2	0.97	2.96	3.281 (2)	145