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2-*tert*-Butyl-6-[(4-chloro-2-nitrophenyl)-diazanyl]-4-methylphenol

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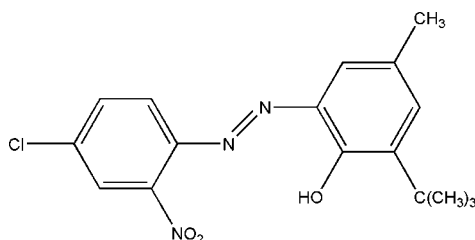
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.044; wR factor = 0.141; data-to-parameter ratio = 16.3.

In the title compound, $\text{C}_{17}\text{H}_{18}\text{ClN}_3\text{O}_3$, the dihedral angle between the planes of the two benzene rings is 1.03 (7)°. The overall conformation of the molecule is influenced, in part, by electron delocalization and by an intramolecular bifurcated $\text{O}-\text{H}\cdots(\text{O},\text{N})$ hydrogen bonds. The O atoms of the nitro group, one of which serves as an H bond acceptor, are disordered over two sets of sites with refined occupancies of 0.56 (3) and 0.44 (3).

Related literature

For benzotriazoles as UV absorbers and their applications in industry, see: Ravichandran *et al.* (2002). *N*-oxides are a key type intermediates in the synthesis of benzotriazoles, see: Wen *et al.* (2006); Crawford (1999). For the use of green synthetic methods to obtain intermediates, see: Tanaka & Toda (2000).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{18}\text{ClN}_3\text{O}_3$ $M_r = 347.79$

Monoclinic, $P2_1/c$
 $a = 14.578$ (4) Å
 $b = 7.0616$ (19) Å
 $c = 17.043$ (5) Å
 $\beta = 101.233$ (3)°
 $V = 1720.9$ (8) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 296$ K
 $0.31 \times 0.18 \times 0.16$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.930$, $T_{\max} = 0.963$

14642 measured reflections
 3927 independent reflections
 2563 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.141$
 $S = 1.03$
 3927 reflections

241 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O3}-\text{H3}\cdots\text{O1}'$	0.82	2.28	2.933 (7)	136
$\text{O3}-\text{H3}\cdots\text{O1}$	0.82	2.50	3.142 (12)	136
$\text{O3}-\text{H3}\cdots\text{N2}$	0.82	1.84	2.553 (2)	145

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); 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: LH2824).

References

- Bruker (2006). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Crawford, J. C. (1999). *Prog. Polym. Sci.* **24**, 7–43.
 Ravichandran, R., Suhadolnik, J., Wood, M. G., Debeillis, A., Detlefsen, R. E., Iyengar, R. & Wolf, J. P. (2002). US Patent No. 6 458 872.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Tanaka, K. & Toda, F. (2000). *Chem. Rev.* **100**, 1025–1074.
 Wen, H.-L., Chen, Y.-H., Hu, H.-W., Zhou, X.-Y. & Liu, C.-B. (2006). *Acta Cryst.* **E62**, o4702–o4703.

supplementary materials

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2-*tert*-Butyl-6-[(4-chloro-2-nitrophenyl)diazenyl]-4-methylphenol

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Comment

Benzotriazoles play an important role as a class of UV absorbers and have promising industrial applications (Ravichandran *et al.*, 2002). N-oxides are a key type intermediates in the synthesis of benzotriazoles (Wen *et al.*, 2006; Crawford, 1999) and the title compound is an important intermediate in the synthesis of 2-(2'-Hydroxy-3'-*tert*-butyl-5'-methylphenyl)-5-chloro benzotriazole (UV 326), a good ultraviolet absorber. Due to the growing awareness of environmental protection, the demand for clean and 'green' (i.e solvent free) chemical syntheses has been growing, so using these synthetic methods to form intermediates have received attention (Tanaka & Toda, 2000). Herein we report a 'green' synthetic method and the crystal structure of the title compound. In the title molecule (Fig. 1) the dihedral angle between the two benzene rings is 1.03 (7)°. The overall conformation of the molecule is influenced, in part, by electron delocalization and by intramolecular O—H···O and O—H···N hydrogen bonds.

Experimental

The title compound was synthesized *via* the solid phase reaction of 4-chloro-2-nitroaniline and 2-*tert*-butyl-4-substituted phenol at room temperature. After intensive grinding a mixture of 4-chloro-2-nitrobenzenamine 1.72 g (10 mmol), 2-*tert*-butyl-4-methylphenol 1.72 g (10.5 mmol), NaNO₂ 0.69 g (10 mmol), and KHSO₄ 1.36 g (10 mmol) in a mortar for 15 min at 293 K, the product was washed with hot water. A few purple crystals suitable for X-ray diffraction analysis were obtained upon recrystallization in ethanol after several days (m. p. 445–446 K), which gave the product in 93% yield and higher than 99% purity (by HPLC).

Refinement

All H atoms were included in calculated positions with O—H = 0.82 Å; C—H(methyl) = 0.96 Å, C—H(aromatic) = 0.93 Å, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}}, \text{O})$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms. The O atoms of the nitro group are disordered over two sites with refined occupancies of 0.56 (3) and 0.44 (3).

Figures

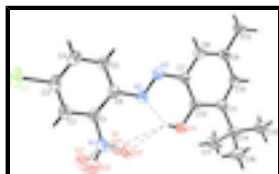


Fig. 1. : The molecular structure of the title compound, showing 30% probability displacement ellipsoids. The minor component of disorder is shown with open bonds and hydrogen bonds are shown with dashed lines.

2-*tert*-Butyl-6-[(4-chloro-2-nitrophenyl)diazenyl]-4-methylphenol

Crystal data

$C_{17}H_{18}ClN_3O_3$	$F_{000} = 728$
$M_r = 347.79$	$D_x = 1.342 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 14.578 (4) \text{ \AA}$	Cell parameters from 4044 reflections
$b = 7.0616 (19) \text{ \AA}$	$\theta = 2.6\text{--}27.2^\circ$
$c = 17.043 (5) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$\beta = 101.233 (3)^\circ$	$T = 296 \text{ K}$
$V = 1720.9 (8) \text{ \AA}^3$	Block, purple
$Z = 4$	$0.31 \times 0.18 \times 0.16 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	3927 independent reflections
Radiation source: fine-focus sealed tube	2563 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.033$
$T = 296 \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -18 \rightarrow 18$
$T_{\text{min}} = 0.930$, $T_{\text{max}} = 0.963$	$k = -9 \rightarrow 8$
14642 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.141$	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.5672P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3927 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
241 parameters	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C11	1.37753 (4)	0.52156 (11)	0.44085 (5)	0.0871 (3)	
O1	0.9625 (4)	0.559 (3)	0.2905 (6)	0.109 (4)	0.56 (3)
O2	1.0758 (7)	0.659 (2)	0.2334 (6)	0.115 (4)	0.56 (3)
O3	0.81516 (9)	0.7932 (3)	0.36241 (8)	0.0666 (5)	
H3	0.8703	0.7643	0.3663	0.100*	
O1'	0.9670 (8)	0.689 (4)	0.2804 (4)	0.100 (5)	0.44 (3)
O2'	1.0687 (12)	0.545 (5)	0.2372 (10)	0.156 (8)	0.44 (3)
N1	1.04252 (15)	0.6167 (4)	0.29115 (12)	0.0765 (6)	
N2	0.98233 (10)	0.7293 (2)	0.43581 (9)	0.0475 (4)	
N3	0.96277 (10)	0.7767 (2)	0.50347 (9)	0.0468 (4)	
C1	1.10633 (13)	0.6202 (3)	0.36932 (12)	0.0528 (5)	
C2	1.19824 (14)	0.5718 (3)	0.36947 (14)	0.0597 (5)	
H2	1.2171	0.5395	0.3221	0.072*	
C3	1.26084 (14)	0.5723 (3)	0.44035 (15)	0.0599 (6)	
C4	1.23301 (14)	0.6162 (3)	0.51114 (14)	0.0606 (5)	
H4	1.2760	0.6122	0.5592	0.073*	
C5	1.14154 (13)	0.6660 (3)	0.51035 (12)	0.0537 (5)	
H5	1.1233	0.6963	0.5582	0.064*	
C6	1.07582 (12)	0.6716 (3)	0.43917 (11)	0.0468 (4)	
C7	0.87202 (12)	0.8321 (3)	0.50305 (10)	0.0425 (4)	
C8	0.85301 (13)	0.8758 (3)	0.57888 (11)	0.0465 (4)	
H8	0.9010	0.8707	0.6236	0.056*	
C9	0.76528 (13)	0.9255 (3)	0.58763 (10)	0.0473 (4)	
C10	0.69528 (13)	0.9379 (3)	0.51815 (11)	0.0485 (5)	
H10	0.6358	0.9748	0.5242	0.058*	
C11	0.70815 (12)	0.8993 (3)	0.44168 (10)	0.0485 (5)	
C12	0.79931 (12)	0.8412 (3)	0.43353 (10)	0.0465 (4)	
C13	0.74126 (16)	0.9610 (4)	0.66868 (11)	0.0646 (6)	
H13A	0.7066	0.8553	0.6831	0.097*	
H13B	0.7042	1.0738	0.6666	0.097*	
H13C	0.7978	0.9763	0.7078	0.097*	
C14	0.62867 (14)	0.9137 (4)	0.36802 (12)	0.0658 (6)	
C15	0.53856 (16)	0.9904 (5)	0.39088 (14)	0.0868 (9)	

supplementary materials

H15A	0.5192	0.9069	0.4290	0.130*
H15B	0.4901	0.9979	0.3439	0.130*
H15C	0.5502	1.1142	0.4139	0.130*
C16	0.65620 (18)	1.0504 (5)	0.30642 (14)	0.0959 (10)
H16A	0.6645	1.1753	0.3290	0.144*
H16B	0.6077	1.0528	0.2594	0.144*
H16C	0.7136	1.0087	0.2924	0.144*
C17	0.60711 (17)	0.7157 (5)	0.33203 (15)	0.0931 (10)
H17A	0.6629	0.6623	0.3190	0.140*
H17B	0.5598	0.7250	0.2844	0.140*
H17C	0.5852	0.6360	0.3701	0.140*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0412 (3)	0.1022 (5)	0.1217 (6)	0.0083 (3)	0.0251 (3)	0.0142 (4)
O1	0.052 (2)	0.186 (11)	0.084 (3)	-0.001 (4)	-0.001 (2)	-0.047 (5)
O2	0.105 (4)	0.185 (9)	0.056 (3)	-0.001 (5)	0.016 (3)	0.012 (4)
O3	0.0420 (7)	0.1165 (13)	0.0417 (7)	0.0091 (8)	0.0094 (6)	-0.0118 (8)
O1'	0.070 (4)	0.173 (13)	0.055 (3)	0.043 (5)	0.007 (2)	-0.013 (4)
O2'	0.115 (7)	0.255 (18)	0.091 (7)	0.062 (10)	0.007 (5)	-0.080 (9)
N1	0.0612 (13)	0.1073 (17)	0.0606 (12)	0.0158 (13)	0.0106 (10)	-0.0208 (12)
N2	0.0388 (8)	0.0553 (10)	0.0491 (9)	-0.0003 (7)	0.0102 (7)	-0.0025 (7)
N3	0.0412 (8)	0.0512 (9)	0.0478 (9)	-0.0017 (7)	0.0083 (7)	-0.0007 (7)
C1	0.0465 (11)	0.0550 (12)	0.0571 (12)	0.0003 (9)	0.0106 (9)	-0.0026 (9)
C2	0.0503 (12)	0.0634 (14)	0.0702 (14)	0.0041 (10)	0.0232 (11)	0.0006 (11)
C3	0.0385 (10)	0.0570 (13)	0.0869 (16)	0.0007 (9)	0.0186 (11)	0.0079 (11)
C4	0.0429 (11)	0.0655 (13)	0.0699 (14)	-0.0021 (9)	0.0021 (10)	0.0061 (11)
C5	0.0455 (11)	0.0588 (12)	0.0561 (12)	-0.0017 (9)	0.0084 (9)	0.0023 (9)
C6	0.0394 (9)	0.0460 (10)	0.0554 (11)	-0.0029 (8)	0.0104 (8)	-0.0006 (8)
C7	0.0374 (9)	0.0472 (10)	0.0425 (9)	-0.0019 (7)	0.0072 (7)	-0.0006 (8)
C8	0.0469 (10)	0.0531 (11)	0.0378 (9)	-0.0022 (8)	0.0038 (8)	0.0008 (8)
C9	0.0515 (11)	0.0542 (11)	0.0380 (9)	-0.0012 (9)	0.0131 (8)	0.0004 (8)
C10	0.0418 (10)	0.0617 (12)	0.0441 (10)	0.0039 (8)	0.0139 (8)	0.0015 (9)
C11	0.0402 (10)	0.0668 (13)	0.0384 (9)	-0.0008 (9)	0.0074 (7)	0.0002 (9)
C12	0.0418 (10)	0.0606 (12)	0.0381 (9)	0.0003 (8)	0.0102 (8)	-0.0032 (8)
C13	0.0651 (13)	0.0909 (17)	0.0408 (10)	0.0048 (12)	0.0178 (10)	-0.0003 (11)
C14	0.0399 (11)	0.115 (2)	0.0415 (10)	0.0116 (11)	0.0065 (8)	-0.0021 (11)
C15	0.0470 (12)	0.156 (3)	0.0552 (13)	0.0292 (15)	0.0053 (10)	0.0027 (15)
C16	0.0679 (16)	0.170 (3)	0.0488 (13)	0.0225 (18)	0.0092 (11)	0.0315 (16)
C17	0.0536 (14)	0.154 (3)	0.0663 (15)	-0.0061 (16)	-0.0019 (11)	-0.0380 (17)

Geometric parameters (\AA , $^\circ$)

C11—C3	1.737 (2)	C8—H8	0.9300
O1—N1	1.233 (8)	C9—C10	1.407 (3)
O2—N1	1.217 (8)	C9—C13	1.511 (2)
O3—C12	1.322 (2)	C10—C11	1.379 (2)
O3—H3	0.8200	C10—H10	0.9300

O1'—N1	1.195 (7)	C11—C12	1.423 (2)
O2'—N1	1.179 (10)	C11—C14	1.537 (3)
N1—C1	1.469 (3)	C13—H13A	0.9600
N2—N3	1.285 (2)	C13—H13B	0.9600
N2—C6	1.413 (2)	C13—H13C	0.9600
N3—C7	1.378 (2)	C14—C17	1.534 (4)
C1—C2	1.382 (3)	C14—C16	1.536 (4)
C1—C6	1.397 (3)	C14—C15	1.540 (3)
C2—C3	1.365 (3)	C15—H15A	0.9600
C2—H2	0.9300	C15—H15B	0.9600
C3—C4	1.381 (3)	C15—H15C	0.9600
C4—C5	1.376 (3)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.392 (3)	C16—H16C	0.9600
C5—H5	0.9300	C17—H17A	0.9600
C7—C8	1.408 (2)	C17—H17B	0.9600
C7—C12	1.429 (3)	C17—H17C	0.9600
C8—C9	1.362 (3)		
C12—O3—H3	109.5	C9—C10—H10	117.5
O2'—N1—O1'	119.6 (10)	C10—C11—C12	116.78 (16)
O2—N1—O1	126.8 (8)	C10—C11—C14	122.62 (17)
O2'—N1—C1	118.1 (7)	C12—C11—C14	120.59 (16)
O1'—N1—C1	122.2 (5)	O3—C12—C11	119.79 (16)
O2—N1—C1	116.6 (5)	O3—C12—C7	120.99 (16)
O1—N1—C1	116.4 (6)	C11—C12—C7	119.20 (15)
N3—N2—C6	114.81 (15)	C9—C13—H13A	109.5
N2—N3—C7	116.74 (15)	C9—C13—H13B	109.5
C2—C1—C6	122.12 (19)	H13A—C13—H13B	109.5
C2—C1—N1	116.10 (18)	C9—C13—H13C	109.5
C6—C1—N1	121.77 (17)	H13A—C13—H13C	109.5
C3—C2—C1	118.8 (2)	H13B—C13—H13C	109.5
C3—C2—H2	120.6	C17—C14—C16	111.1 (2)
C1—C2—H2	120.6	C17—C14—C11	109.2 (2)
C2—C3—C4	120.94 (19)	C16—C14—C11	110.12 (19)
C2—C3—C11	119.29 (17)	C17—C14—C15	107.7 (2)
C4—C3—C11	119.75 (18)	C16—C14—C15	107.5 (2)
C5—C4—C3	119.8 (2)	C11—C14—C15	111.17 (17)
C5—C4—H4	120.1	C14—C15—H15A	109.5
C3—C4—H4	120.1	C14—C15—H15B	109.5
C4—C5—C6	121.11 (19)	H15A—C15—H15B	109.5
C4—C5—H5	119.4	C14—C15—H15C	109.5
C6—C5—H5	119.4	H15A—C15—H15C	109.5
C5—C6—C1	117.11 (17)	H15B—C15—H15C	109.5
C5—C6—N2	122.56 (17)	C14—C16—H16A	109.5
C1—C6—N2	120.32 (17)	C14—C16—H16B	109.5
N3—C7—C8	114.70 (16)	H16A—C16—H16B	109.5
N3—C7—C12	124.97 (16)	C14—C16—H16C	109.5
C8—C7—C12	120.30 (16)	H16A—C16—H16C	109.5
C9—C8—C7	120.93 (17)	H16B—C16—H16C	109.5

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C9—C8—H8	119.5	C14—C17—H17A	109.5
C7—C8—H8	119.5	C14—C17—H17B	109.5
C8—C9—C10	117.79 (16)	H17A—C17—H17B	109.5
C8—C9—C13	122.19 (17)	C14—C17—H17C	109.5
C10—C9—C13	120.00 (17)	H17A—C17—H17C	109.5
C11—C10—C9	124.95 (17)	H17B—C17—H17C	109.5
C11—C10—H10	117.5		
C6—N2—N3—C7	-179.36 (15)	N2—N3—C7—C8	177.70 (16)
O2'—N1—C1—C2	12 (2)	N2—N3—C7—C12	-0.3 (3)
O1'—N1—C1—C2	-165.3 (16)	N3—C7—C8—C9	-177.44 (18)
O2—N1—C1—C2	-32.9 (10)	C12—C7—C8—C9	0.7 (3)
O1—N1—C1—C2	142.5 (11)	C7—C8—C9—C10	-2.1 (3)
O2'—N1—C1—C6	-168 (2)	C7—C8—C9—C13	176.00 (19)
O1'—N1—C1—C6	14.0 (16)	C8—C9—C10—C11	1.5 (3)
O2—N1—C1—C6	146.4 (10)	C13—C9—C10—C11	-176.6 (2)
O1—N1—C1—C6	-38.2 (11)	C9—C10—C11—C12	0.6 (3)
C6—C1—C2—C3	0.7 (3)	C9—C10—C11—C14	179.5 (2)
N1—C1—C2—C3	-179.9 (2)	C10—C11—C12—O3	176.69 (19)
C1—C2—C3—C4	1.4 (3)	C14—C11—C12—O3	-2.2 (3)
C1—C2—C3—C11	-177.30 (16)	C10—C11—C12—C7	-2.0 (3)
C2—C3—C4—C5	-2.0 (3)	C14—C11—C12—C7	179.05 (19)
C11—C3—C4—C5	176.67 (17)	N3—C7—C12—O3	0.7 (3)
C3—C4—C5—C6	0.5 (3)	C8—C7—C12—O3	-177.22 (18)
C4—C5—C6—C1	1.5 (3)	N3—C7—C12—C11	179.40 (18)
C4—C5—C6—N2	-177.41 (19)	C8—C7—C12—C11	1.5 (3)
C2—C1—C6—C5	-2.1 (3)	C10—C11—C14—C17	-114.1 (2)
N1—C1—C6—C5	178.6 (2)	C12—C11—C14—C17	64.7 (3)
C2—C1—C6—N2	176.80 (19)	C10—C11—C14—C16	123.6 (2)
N1—C1—C6—N2	-2.5 (3)	C12—C11—C14—C16	-57.5 (3)
N3—N2—C6—C5	0.2 (3)	C10—C11—C14—C15	4.6 (3)
N3—N2—C6—C1	-178.68 (17)	C12—C11—C14—C15	-176.6 (2)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots O1'	0.82	2.28	2.933 (7)	136
O3—H3 \cdots O1	0.82	2.50	3.142 (12)	136
O3—H3 \cdots N2	0.82	1.84	2.553 (2)	145

Fig. 1

