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1-Benzyl-1*H*-benzotriazole 3-oxide–1-hydroxy-1*H*-benzotriazole (1/1)

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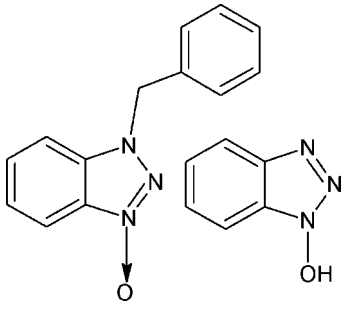
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.132; data-to-parameter ratio = 13.0.

In the title compound, $C_6H_5N_3O\cdot C_{13}H_{11}N_3O$, the benzotriazole ring system in the 1-benzyl-1*H*-benzotriazole 3-oxide (*A*) molecule is close to being planar (r.m.s. deviation = 0.011 Å); its mean plane forms a dihedral angle of 67.56 (7)° with that of the attached phenyl ring. The benzotriazole ring system in the 1-hydroxybenzotriazole (*B*) molecule is also close to being planar (r.m.s. deviation = 0.010 Å). In the crystal, weak C—H···O and C—H···π interactions are present. The *A* and *B* molecules are linked by an O—H···N hydrogen bond.

Related literature

For related structures and background to benzotriazoles, see: Ravindran *et al.* (2009); Selvarathy Grace *et al.* (2012).



Experimental

Crystal data

$C_6H_5N_3O\cdot C_{13}H_{11}N_3O$
M_r = 360.38
Monoclinic, $P2_1/c$
a = 11.2728 (8) Å
b = 12.2354 (5) Å
c = 13.1002 (9) Å
β = 110.946 (3)°
V = 1687.47 (18) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 193 K
0.40 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
3364 measured reflections
3197 independent reflections
2980 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
3 standard reflections every 60 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.132
S = 1.08
3197 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N3^{i}	0.84	2.57	3.3621 (18)	157
C3—H3···O1^{ii}	0.95	2.50	3.200 (2)	130
C7—H7B···$Cg1^{iii}$	0.99	2.85	3.5146 (17)	125
C18—H18···$Cg1^{iv}$	0.95	2.69	3.510 (2)	145

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971; Wiehl & Schollmeyer, 1994); 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: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6878).

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Selvarathy Grace, P., Jebas, S. R., Ravindran Durai Nayagam, B. & Schollmeyer, D. (2012). *Acta Cryst.* E**68**, o1132.
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supporting information

Acta Cryst. (2012). E**68**, o2399 [https://doi.org/10.1107/S1600536812030061]

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S1. Comment

As part of our ongoing studies of benzotriazole derivatives (Ravindran *et al.*, 2009; Selvarathy Grace *et al.*, 2012), we now report the crystal structure of the title compound (I), (Fig. 1).

The benzotriazole rings are essentially planar with the maximum deviation from planarity being 0.015 (14) Å for atoms N1 and N5. The mean plane of the benzotriazole ring N1—N3/C1—C6 forms a dihedral angle of 67.56 (7) Å with the mean plane of the phenyl ring (C8—C13).

The crystal packing features weak C—H···π interactions. The hydrogen bonding interactions are shown in Fig 2.

S2. Experimental

A mixture of the sodium salt of 1- hydroxyl benzotriazole (0.314 g, 2 mmol) and benzyl chloride (0.126 g, 1 mmol) in methanol (10 ml), were heated at 333K with stirring for 6 hours. The mixture was kept aside for slow evaporation. After a week, colourless blocks were recovered.

S3. Refinement

H atoms were positioned geometrically [C—H = 0.95 (aromatic) or 0.99 Å (methylene)] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

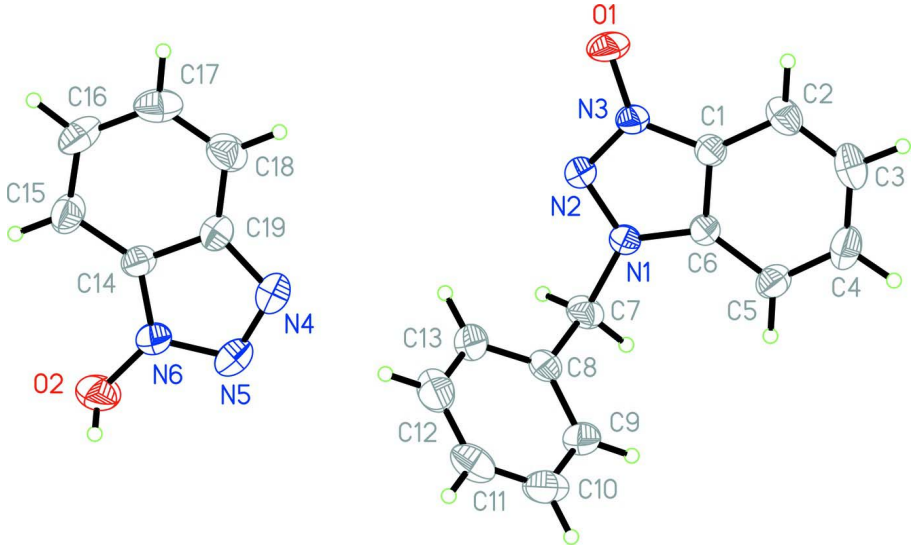

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level.

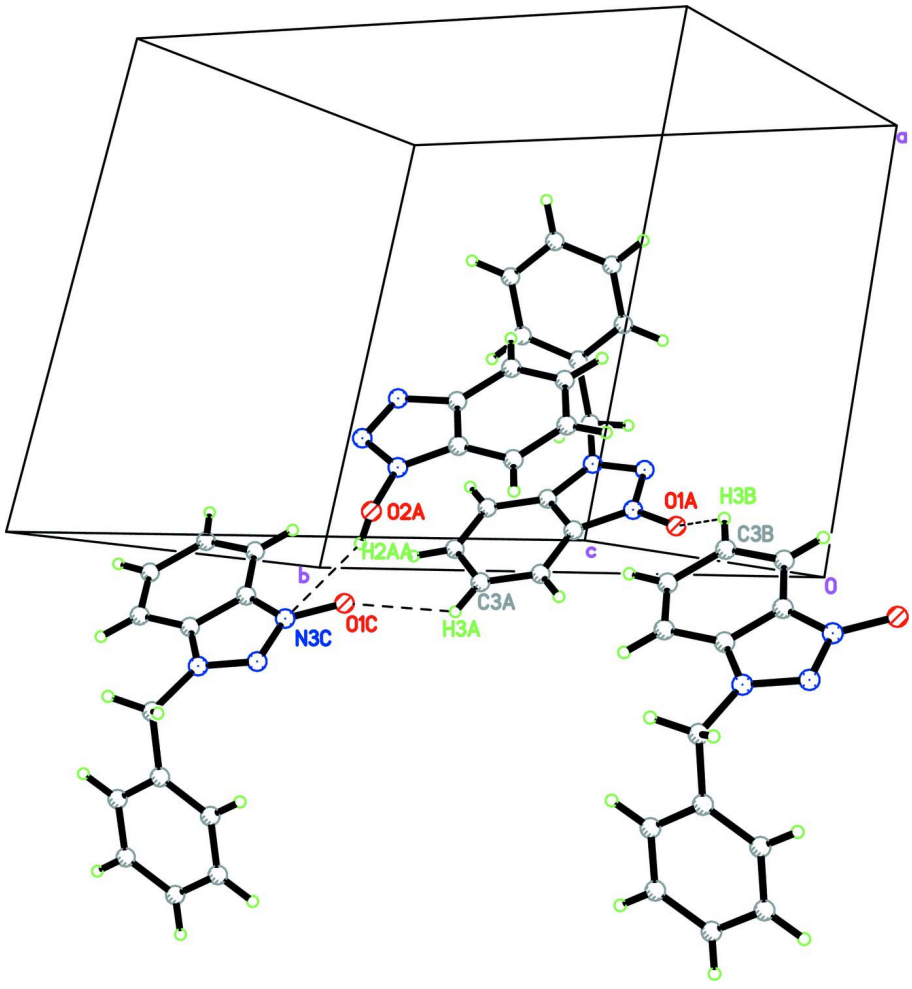

Figure 2

The unit cell showing the hydrogen bonding interaction of the title compound. Hydrogen bonds are shown as dashed lines.

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Crystal data

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$c = 13.1002\ (9)$ Å
$\beta = 110.946\ (3)°$
$V = 1687.47\ (18)$ Å^3
$Z = 4$

$F(000) = 752$
$D_x = 1.419$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 65–69°$
$\mu = 0.80$ mm^{-1}
$T = 193$ K
Block, colourless
0.40 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: rotating anode
Graphite monochromator
$\omega/2\theta$ scans
3364 measured reflections
3197 independent reflections
2980 reflections with $I > 2\sigma(I)$
$R_{int} = 0.102$
$\theta_{max} = 70.0°$, $\theta_{min} = 4.2°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 14$
$l = -15 \rightarrow 14$
3 standard reflections every 60 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.132$
$S = 1.08$
3197 reflections
245 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
$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.6089P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0035 (5)

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 $F^2 > 2$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}
N1	0.23017 (11)	0.44814 (10)	0.07382 (10)	0.0233 (3)
N2	0.21688 (11)	0.34031 (10)	0.08272 (10)	0.0261 (3)
N3	0.12730 (11)	0.32935 (10)	0.12460 (10)	0.0256 (3)
C1	0.08113 (13)	0.42800 (12)	0.14320 (11)	0.0231 (3)
C2	−0.01438 (14)	0.45549 (14)	0.18361 (13)	0.0314 (4)
H2	−0.0618	0.4017	0.2048	0.038*
C3	−0.03466 (15)	0.56486 (15)	0.19043 (13)	0.0351 (4)
H3	−0.0985	0.5880	0.2172	0.042*
C4	0.03627 (15)	0.64472 (14)	0.15895 (13)	0.0340 (4)
H4	0.0191	0.7197	0.1663	0.041*
C5	0.12920 (14)	0.61800 (12)	0.11806 (13)	0.0284 (3)
H5	0.1760	0.6719	0.0963	0.034*
C6	0.15024 (13)	0.50592 (11)	0.11070 (11)	0.0216 (3)
C7	0.32424 (14)	0.48951 (13)	0.02917 (12)	0.0285 (3)
H7A	0.2976	0.5627	−0.0030	0.034*

H7B	0.3269	0.4402	−0.0299	0.034*
C8	0.45521 (13)	0.49730 (12)	0.11541 (12)	0.0250 (3)
C9	0.50482 (15)	0.59795 (13)	0.15887 (14)	0.0327 (4)
H9	0.4566	0.6626	0.1333	0.039*
C10	0.62432 (17)	0.60451 (15)	0.23944 (15)	0.0384 (4)
H10	0.6576	0.6736	0.2691	0.046*
C11	0.69520 (15)	0.51109 (15)	0.27686 (13)	0.0368 (4)
H11	0.7768	0.5158	0.3326	0.044*
C12	0.64695 (16)	0.41032 (15)	0.23292 (15)	0.0379 (4)
H12	0.6957	0.3459	0.2583	0.045*
C13	0.52801 (15)	0.40353 (13)	0.15226 (14)	0.0323 (4)
H13	0.4957	0.3345	0.1217	0.039*
O1	0.09227 (11)	0.23257 (9)	0.14562 (11)	0.0383 (3)
N4	0.66756 (14)	0.18397 (12)	0.08895 (14)	0.0428 (4)
N5	0.75634 (14)	0.21667 (11)	0.05304 (14)	0.0417 (4)
N6	0.81861 (13)	0.12778 (10)	0.03929 (12)	0.0312 (3)
C14	0.77039 (14)	0.03437 (12)	0.06416 (12)	0.0252 (3)
C15	0.79910 (16)	−0.07638 (13)	0.06063 (13)	0.0329 (4)
H15	0.8655	−0.1009	0.0377	0.039*
C16	0.72455 (18)	−0.14724 (13)	0.09268 (14)	0.0372 (4)
H16	0.7400	−0.2235	0.0921	0.045*
C17	0.62562 (17)	−0.11034 (15)	0.12655 (14)	0.0378 (4)
H17	0.5768	−0.1625	0.1482	0.045*
C18	0.59823 (16)	−0.00226 (15)	0.12905 (14)	0.0353 (4)
H18	0.5313	0.0218	0.1516	0.042*
C19	0.67306 (15)	0.07221 (13)	0.09693 (13)	0.0293 (3)
O2	0.91290 (12)	0.13654 (10)	−0.00258 (11)	0.0419 (3)
H2A	0.9753	0.1692	0.0424	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0237 (6)	0.0214 (6)	0.0286 (6)	−0.0013 (5)	0.0138 (5)	0.0007 (5)
N2	0.0253 (6)	0.0211 (6)	0.0344 (7)	−0.0006 (5)	0.0139 (5)	−0.0006 (5)
N3	0.0235 (6)	0.0201 (6)	0.0339 (7)	−0.0012 (4)	0.0112 (5)	0.0047 (5)
C1	0.0217 (6)	0.0232 (7)	0.0246 (7)	0.0012 (5)	0.0086 (5)	0.0035 (5)
C2	0.0267 (7)	0.0391 (9)	0.0321 (8)	0.0020 (6)	0.0150 (6)	0.0055 (7)
C3	0.0309 (8)	0.0452 (10)	0.0327 (8)	0.0095 (7)	0.0157 (7)	−0.0010 (7)
C4	0.0361 (8)	0.0288 (8)	0.0355 (8)	0.0080 (6)	0.0109 (7)	−0.0055 (6)
C5	0.0311 (8)	0.0215 (7)	0.0322 (8)	−0.0004 (6)	0.0108 (6)	0.0006 (6)
C6	0.0210 (6)	0.0215 (7)	0.0226 (7)	0.0002 (5)	0.0081 (5)	0.0004 (5)
C7	0.0290 (8)	0.0327 (8)	0.0294 (8)	−0.0041 (6)	0.0173 (6)	0.0016 (6)
C8	0.0264 (7)	0.0273 (7)	0.0280 (7)	−0.0023 (6)	0.0179 (6)	0.0000 (6)
C9	0.0350 (8)	0.0258 (8)	0.0426 (9)	−0.0038 (6)	0.0203 (7)	0.0017 (6)
C10	0.0405 (9)	0.0372 (9)	0.0416 (9)	−0.0148 (7)	0.0197 (7)	−0.0068 (7)
C11	0.0292 (8)	0.0537 (11)	0.0301 (8)	−0.0065 (7)	0.0138 (6)	0.0012 (7)
C12	0.0342 (8)	0.0414 (9)	0.0415 (9)	0.0066 (7)	0.0177 (7)	0.0076 (7)
C13	0.0334 (8)	0.0287 (8)	0.0407 (9)	0.0001 (6)	0.0206 (7)	−0.0030 (6)

O1	0.0371 (6)	0.0216 (6)	0.0573 (8)	−0.0058 (4)	0.0181 (5)	0.0105 (5)
N4	0.0421 (8)	0.0264 (7)	0.0647 (10)	0.0033 (6)	0.0249 (7)	−0.0049 (7)
N5	0.0449 (8)	0.0207 (7)	0.0623 (10)	0.0006 (6)	0.0225 (7)	0.0008 (6)
N6	0.0332 (7)	0.0223 (6)	0.0432 (8)	−0.0021 (5)	0.0199 (6)	0.0021 (5)
C14	0.0301 (7)	0.0211 (7)	0.0261 (7)	−0.0034 (6)	0.0121 (6)	−0.0010 (5)
C15	0.0427 (9)	0.0258 (8)	0.0357 (8)	0.0037 (7)	0.0208 (7)	−0.0014 (6)
C16	0.0550 (11)	0.0203 (7)	0.0382 (9)	−0.0034 (7)	0.0189 (8)	−0.0006 (6)
C17	0.0452 (10)	0.0367 (9)	0.0342 (9)	−0.0141 (7)	0.0175 (7)	0.0008 (7)
C18	0.0343 (8)	0.0419 (9)	0.0350 (9)	−0.0054 (7)	0.0187 (7)	−0.0043 (7)
C19	0.0313 (8)	0.0247 (8)	0.0327 (8)	0.0001 (6)	0.0124 (6)	−0.0043 (6)
O2	0.0451 (7)	0.0395 (7)	0.0521 (7)	−0.0101 (5)	0.0309 (6)	−0.0005 (6)

Geometric parameters (Å, º)

N1—N2	1.3376 (17)	C10—H10	0.9500
N1—C6	1.3625 (18)	C11—C12	1.387 (3)
N1—C7	1.4718 (17)	C11—H11	0.9500
N2—N3	1.3171 (17)	C12—C13	1.381 (2)
N3—O1	1.3082 (16)	C12—H12	0.9500
N3—C1	1.3703 (19)	C13—H13	0.9500
C1—C6	1.391 (2)	N4—N5	1.311 (2)
C1—C2	1.400 (2)	N4—C19	1.371 (2)
C2—C3	1.366 (2)	N5—N6	1.3411 (19)
C2—H2	0.9500	N6—C14	1.3545 (19)
C3—C4	1.414 (3)	N6—O2	1.3635 (17)
C3—H3	0.9500	C14—C19	1.393 (2)
C4—C5	1.376 (2)	C14—C15	1.398 (2)
C4—H4	0.9500	C15—C16	1.373 (2)
C5—C6	1.401 (2)	C15—H15	0.9500
C5—H5	0.9500	C16—C17	1.414 (3)
C7—H7A	0.9900	C16—H16	0.9500
C7—H7B	0.9900	C17—C18	1.361 (3)
C8—C9	1.388 (2)	C17—H17	0.9500
C8—C13	1.393 (2)	C18—C19	1.404 (2)
C9—H9	0.9500	C18—H18	0.9500
C10—C11	1.380 (3)	O2—H2A	0.8400
N2—N1—C6	111.83 (11)	C11—C10—C9	120.30 (16)
N2—N1—C7	119.53 (12)	C11—C10—H10	119.9
C6—N1—C7	128.63 (12)	C9—C10—H10	119.9
N3—N2—N1	105.26 (11)	C10—C11—C12	119.83 (16)
O1—N3—N2	120.92 (12)	C10—C11—H11	120.1
O1—N3—C1	126.69 (12)	C12—C11—H11	120.1
N2—N3—C1	112.38 (12)	C13—C12—C11	120.02 (16)
N3—C1—C6	105.04 (12)	C13—C12—H12	120.0
N3—C1—C2	132.16 (14)	C11—C12—H12	120.0
C6—C1—C2	122.80 (14)	C12—C13—C8	120.41 (15)
C3—C2—C1	115.44 (15)	C12—C13—H13	119.8

C3—C2—H2	122.3	C8—C13—H13	119.8
C1—C2—H2	122.3	N5—N4—C19	108.20 (14)
C2—C3—C4	122.17 (15)	N4—N5—N6	107.69 (13)
C2—C3—H3	118.9	N5—N6—C14	112.19 (13)
C4—C3—H3	118.9	N5—N6—O2	120.74 (13)
C5—C4—C3	122.55 (15)	C14—N6—O2	126.92 (13)
C5—C4—H4	118.7	N6—C14—C19	102.81 (13)
C3—C4—H4	118.7	N6—C14—C15	133.83 (14)
C4—C5—C6	115.51 (14)	C19—C14—C15	123.35 (14)
C4—C5—H5	122.2	C16—C15—C14	115.32 (15)
C6—C5—H5	122.2	C16—C15—H15	122.3
N1—C6—C1	105.47 (12)	C14—C15—H15	122.3
N1—C6—C5	133.00 (14)	C15—C16—C17	122.14 (15)
C1—C6—C5	121.52 (13)	C15—C16—H16	118.9
N1—C7—C8	112.06 (12)	C17—C16—H16	118.9
N1—C7—H7A	109.2	C18—C17—C16	121.94 (16)
C8—C7—H7A	109.2	C18—C17—H17	119.0
N1—C7—H7B	109.2	C16—C17—H17	119.0
C8—C7—H7B	109.2	C17—C18—C19	117.22 (15)
H7A—C7—H7B	107.9	C17—C18—H18	121.4
C9—C8—C13	119.20 (14)	C19—C18—H18	121.4
C9—C8—C7	120.43 (14)	N4—C19—C14	109.10 (14)
C13—C8—C7	120.37 (14)	N4—C19—C18	130.86 (15)
C10—C9—C8	120.23 (15)	C14—C19—C18	120.03 (15)
C10—C9—H9	119.9	N6—O2—H2A	109.5
C8—C9—H9	119.9		

C6—N1—N2—N3	0.52 (15)	C7—C8—C9—C10	178.88 (14)
C7—N1—N2—N3	179.96 (12)	C8—C9—C10—C11	0.2 (3)
N1—N2—N3—O1	−178.89 (12)	C9—C10—C11—C12	0.5 (3)
N1—N2—N3—C1	0.15 (16)	C10—C11—C12—C13	−0.3 (3)
O1—N3—C1—C6	178.25 (13)	C11—C12—C13—C8	−0.7 (2)
N2—N3—C1—C6	−0.73 (16)	C9—C8—C13—C12	1.5 (2)
O1—N3—C1—C2	−2.6 (3)	C7—C8—C13—C12	−178.64 (14)
N2—N3—C1—C2	178.37 (15)	C19—N4—N5—N6	−0.6 (2)
N3—C1—C2—C3	−179.72 (15)	N4—N5—N6—C14	1.1 (2)
C6—C1—C2—C3	−0.8 (2)	N4—N5—N6—O2	176.88 (14)
C1—C2—C3—C4	−0.1 (2)	N5—N6—C14—C19	−1.03 (18)
C2—C3—C4—C5	0.9 (3)	O2—N6—C14—C19	−176.51 (14)
C3—C4—C5—C6	−0.7 (2)	N5—N6—C14—C15	178.09 (17)
N2—N1—C6—C1	−0.96 (15)	O2—N6—C14—C15	2.6 (3)
C7—N1—C6—C1	179.66 (13)	N6—C14—C15—C16	−179.35 (17)
N2—N1—C6—C5	−179.96 (15)	C19—C14—C15—C16	−0.4 (2)
C7—N1—C6—C5	0.7 (3)	C14—C15—C16—C17	0.1 (2)
N3—C1—C6—N1	0.98 (15)	C15—C16—C17—C18	0.2 (3)
C2—C1—C6—N1	−178.23 (13)	C16—C17—C18—C19	−0.3 (3)
N3—C1—C6—C5	−179.87 (13)	N5—N4—C19—C14	−0.01 (19)
C2—C1—C6—C5	0.9 (2)	N5—N4—C19—C18	−178.73 (17)

C4—C5—C6—N1	178.71 (15)	N6—C14—C19—N4	0.61 (17)
C4—C5—C6—C1	−0.2 (2)	C15—C14—C19—N4	−178.63 (15)
C6—N1—C7—C8	94.88 (17)	N6—C14—C19—C18	179.50 (14)
N1—C7—C8—C9	−104.04 (16)	C15—C14—C19—C18	0.3 (2)
N1—C7—C8—C13	76.11 (17)	C17—C18—C19—N4	178.71 (17)
C13—C8—C9—C10	−1.3 (2)	C17—C18—C19—C14	0.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N3^{i}	0.84	2.57	3.3621 (18)	157
C3—H3···O1^{ii}	0.95	2.50	3.200 (2)	130
C7—H7*B*···*Cg*1^{iii}	0.99	2.85	3.5146 (17)	125
C18—H18···*Cg*1^{iv}	0.95	2.69	3.510 (2)	145

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+1, *y*−1/2, −*z*+1/2.