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17-Hydroxy-1,8-dimethyl-17-azapentacyclo[6.6.5.0^{2,7}.0^{9,14}.0^{15,19}]nonadeca-2,4,6,9(14),10,12-hexaene-16,18-dione

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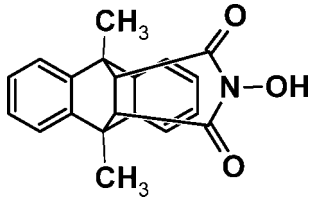
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.096; data-to-parameter ratio = 12.7.

In the title compound, $C_{20}H_{17}NO_3$ (alternative name: *N*-hydroxy-9,10-dimethyl-9,10-ethanoanthracene-11,12-dicarboximide), the rigid ethanoanthracene-dicarboximide moiety has a roof-shaped geometry, the interplanar angle between the two terminal phenyl rings being 124.9 (6)°. In the crystal, molecules are linked *via* O—H···O hydrogen bonds, forming chains along [010]. C—H···O and C—H···π interactions link adjacent chains, leading to the formation of a three-dimensional structure.

Related literature

For the synthesis of the title compound, see: Kossakowski & Jarocka (2000). For the biological activity of related compounds, see: Bova *et al.* (2009). For related structures, see: Atherton & Jones (2002); Smet *et al.* (2000); Su *et al.* (2011), Guo *et al.* (2010); Adams *et al.* (2006); He & Ng (2007); Weber *et al.* (1991, 1994); Yang & Swager (1998). The rigid ethanoanthracenedicarboximide moiety of the title compound shows the typical roof-shaped geometry (Weber *et al.*, 1991; Csöregh *et al.*, 2003). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$C_{20}H_{17}NO_3$
M_r = 319.36
Monoclinic, $P2_1/n$
a = 13.904 (1) Å
b = 8.104 (1) Å
c = 13.946 (1) Å
β = 97.39 (1)°
V = 1558.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.40 × 0.40 × 0.30 mm

Data collection

Oxford Diffraction Xcalibur (Sapphire2) diffractometer
5321 measured reflections
2827 independent reflections
2467 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.04
2827 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C6–C11 ring. *Cg*2 refers to the mid-point of the C15—C16 bond.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1^{i}	0.96 (2)	1.69 (2)	2.630 (1)	167 (2)
C8—H8···O1^{ii}	0.95	2.54	3.408 (2)	152
C15—H15···O3^{iii}	0.95	2.46	3.273 (2)	143
C17—H17···O2^{iv}	0.95	2.54	3.457 (2)	163
C4—H4···*Cg*1^{v}	1.00	2.66	3.518 (3)	144
C10—H10···*Cg*2^{vi}	0.95	2.77	3.668 (3)	158

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $x, y+1, z$; (v) $-x, -y+1, -z+1$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: *publCIF*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2475).

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supplementary materials

Acta Cryst. (2012). E**68**, o3293–o3294 [doi:10.1107/S1600536812045151]

17-Hydroxy-1,8-dimethyl-17-azapentacyclo-[6.6.5.$0^{2,7}$.$0^{9,14}$.$0^{15,19}$]nonadeca-2,4,6,9(14),10,12-hexaene-16,18-dione

Barbara Miroslaw, Anna E. Koziol, Magdalena Pakosinska-Parys and Marta Struga

Comment

Roof-shaped aromatic hydrocarbon derivatives have been used for inclusion of neutral compounds (Weber *et al.*, 1991; 1994) and as porous polymer films and sensors for dinitrotoluene with possible application as a land mine detectors (Yang & Swager, 1998). The *N*-substitution is the most common way of modification of these molecules (Weber *et al.*, 1994; Smet *et al.*, 2000). Some experiments were also conducted on the substitution in the aryl moiety (Atherton & Jones, 2002; Adams *et al.*, 2006; He & Ng, 2007). The search of the CSD (CSD v5.33 and updates; Allen, 2002) revealed 67 crystal structures of compounds with the rigid pentacyclic 9,10-ethanoanthracenedicarboximide skeleton. However, none of these derivatives has *N*-hydroxy substituent and only two molecules are symmetrically substituted at bridgehead C atoms (here C5, C12; see Fig. 1). In these crystals the polycyclic skeletons are combined with voluminous macrocyclic fragments. (Su *et al.*, 2011; Guo *et al.*, 2010). The rigid ethanoanthracenedicarboximide moiety of the title compound (Fig. 1) shows the typical roof-shaped geometry (Weber *et al.*, 1991; Csöregh *et al.*, 2003); the interplanar angle between the two terminal phenyl rings is 124.9 °. The hydroxyl O atom interacts through the O3–H···O1 hydrogen bond (Fig. 2). Molecules form chains along the 2_1 screw axis. Between adjacent chains many C–H···O and C–H···π interactions are observed (Figs. 2–4, Table 1).

Experimental

The title compound, UPAC name: 17-hydroxy-1,8-dimethyl-17-azapentacyclo-[6.6.5.$0^{2,7}$.$0^{9,14}$.$0^{15,19}$]nonadeca-2,4,6,9(14),10,12-hexaene-16,18-dione, was synthesized in the search of compounds with potential anxiolytic activity, as described previously (Kossakowski & Jarocka, 2000).

Refinement

All C-bonded H atoms were positioned geometrically and allowed to ride on the attached atom with the C—H bond lengths of 0.95 Å for aromatic atoms, 1.00 Å for methine and 0.98 Å for methyl groups. U_{iso}(H) values were fixed to 1.2U_{eq}(C) and 1.5U_{eq}(C_{methyl}). The hydroxyl H atom was located in the difference electron density map and refined isotropically.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); 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: *publCIF*.

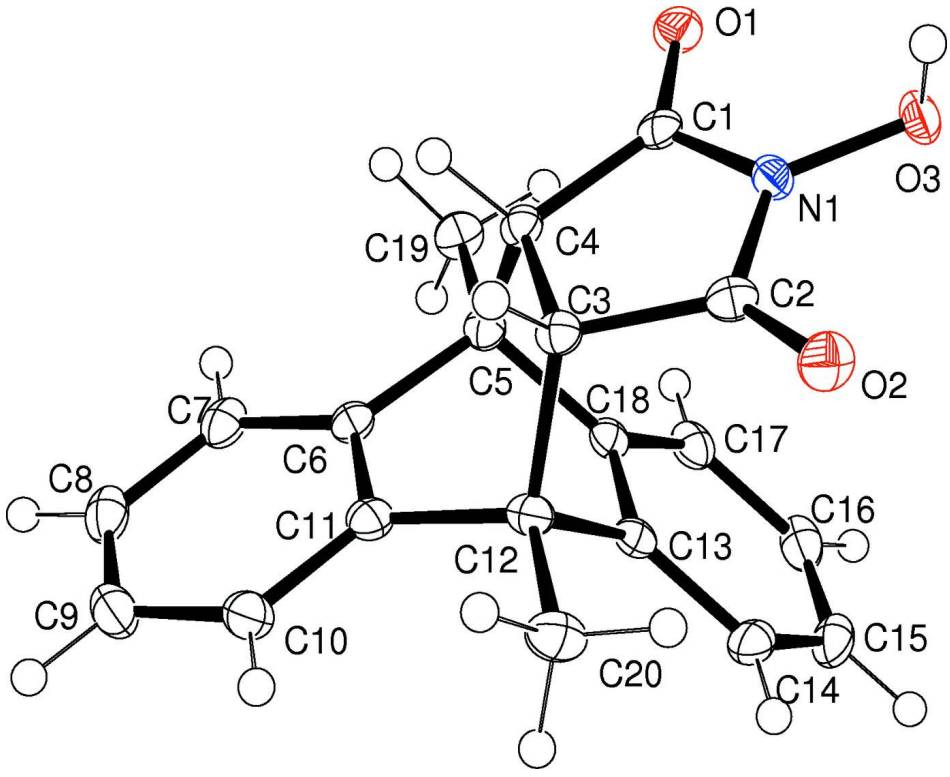

Figure 1

Ortep view of the title compound with atom numbering scheme. Ellipsoids for non-hydrogen atoms were drawn at the 50 % probability level.

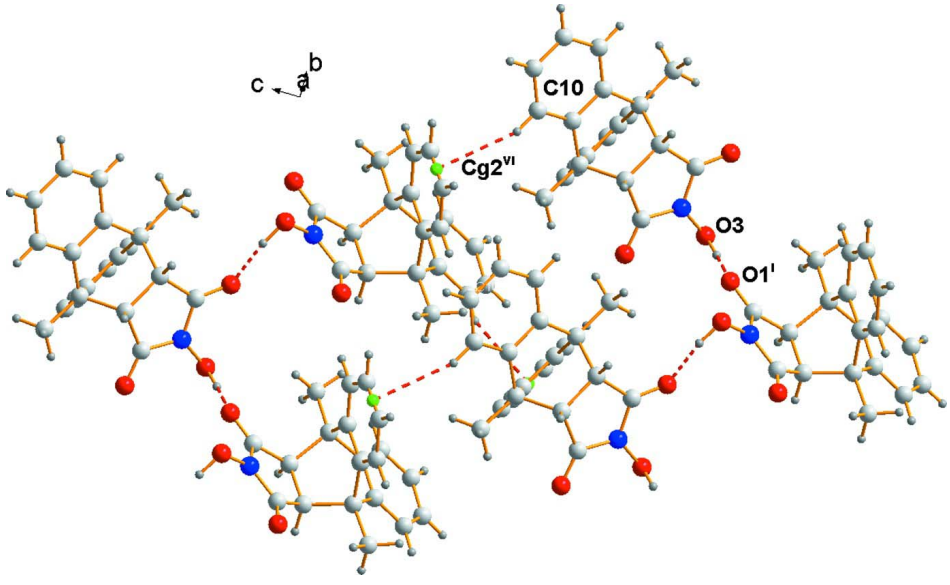

Figure 2

Linear association of molecules in crystal of 1 through the O–H···O hydrogen bonds and C–H···π interactions between adjacent chains. The Cg2 refers to the center of gravity between atoms C15/C16. Symmetry codes: (i) –*x*+1/2, *y*–1/2, –*z*+3/2; (vi) –*x*+1/2, *y*–1/2, –*z*+1/2.

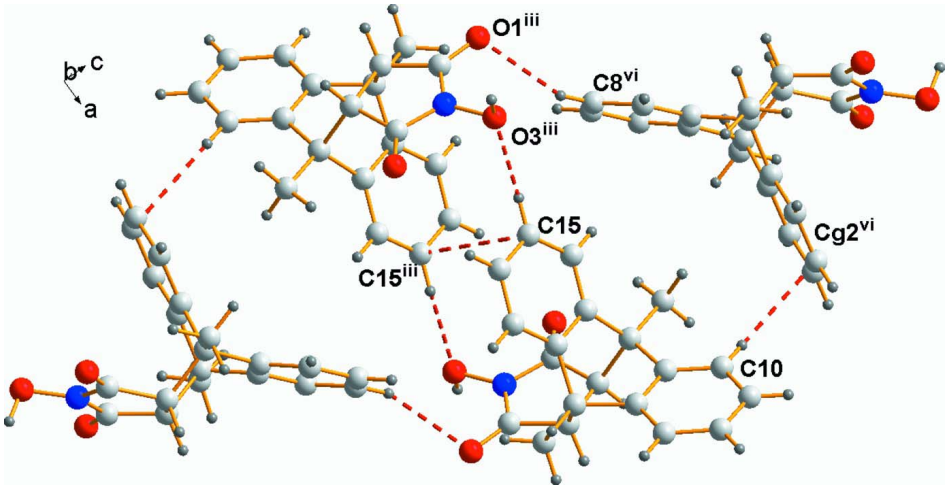

Figure 3

C–H···O and C–H···π interactions in crystal of 1 with short C15···C15^{iii} intermolecular contact (3.386 (2) Å). The Cg2 is the centroid of the C15/C16 bond. Symmetry codes: (iii) –*x*+1, –*y*+1, –*z*+1; (vi) –*x*+1/2, *y*–1/2, –*z*+1/2.

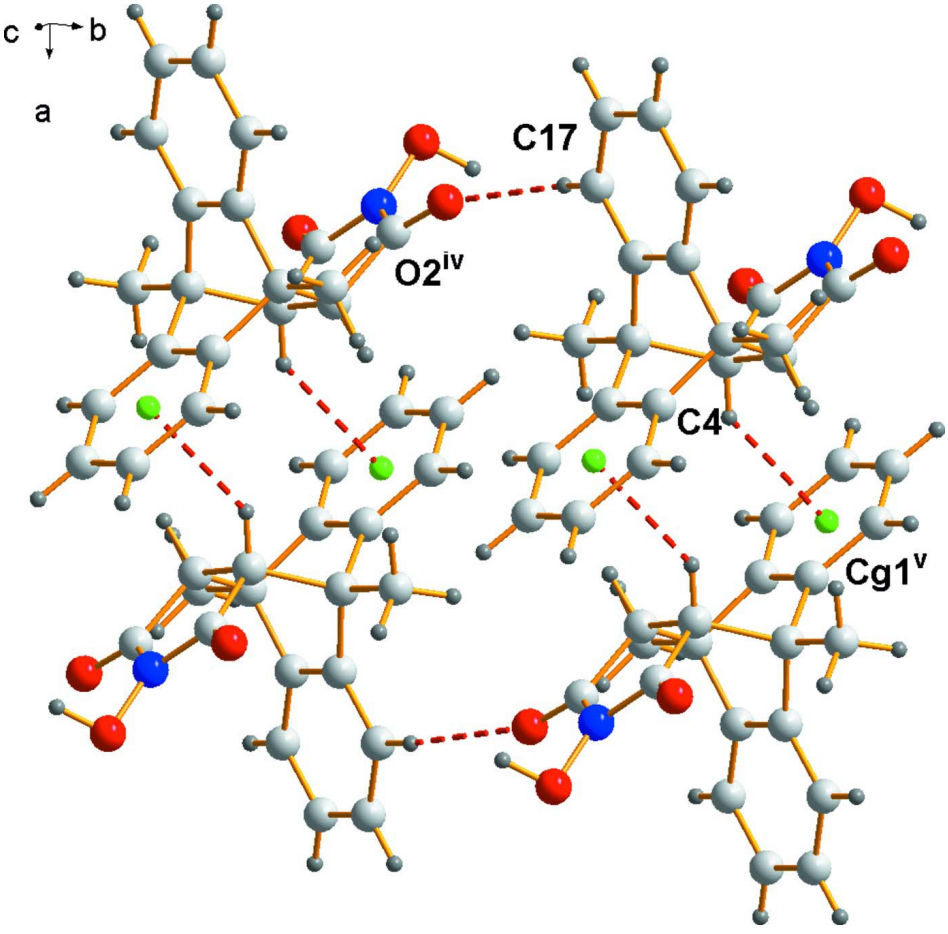

Figure 4

C–H···O hydrogen bonds and C–H···π interactions in crystal of 1. The Cg1 refers to the centroid of the C6–C11 ring. Symmetry codes: (iv) *x*, *y*+1, *z*; (v) –*x*, –*y*+1, –*z*+1.

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Crystal data

$C_{20}H_{17}NO_3$
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Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.904 (1) Å
b = 8.104 (1) Å
c = 13.946 (1) Å
β = 97.39 (1)°
V = 1558.4 (3) Å^3
Z = 4
$F(000)$ = 672
D_x = 1.361 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3666 reflections
θ = 2.9–29.8°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colourless
0.40 × 0.40 × 0.30 mm

Data collection

Oxford Diffraction Xcalibur (Sapphire2) diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 8.4221 pixels mm^{-1}
ω scans
5321 measured reflections
2827 independent reflections
2467 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.2°, θ_{min} = 2.9°
h = −16→16
k = −9→6
l = −9→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.04
2827 reflections
223 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.4721P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.28230 (8)	0.37858 (13)	0.63969 (8)	0.0154 (3)
O1	0.23524 (7)	0.61166 (12)	0.71225 (6)	0.0201 (2)
O2	0.30265 (7)	0.15262 (11)	0.54480 (7)	0.0217 (2)
O3	0.36001 (7)	0.34569 (12)	0.70937 (7)	0.0194 (2)
H3A	0.3338 (15)	0.258 (3)	0.7443 (15)	0.049 (6)*
C1	0.22513 (9)	0.51497 (16)	0.64443 (9)	0.0148 (3)
C2	0.25875 (10)	0.27735 (16)	0.55890 (9)	0.0161 (3)

C3	0.17056 (9)	0.35563 (16)	0.49956 (9)	0.0151 (3)
H3	0.1129	0.2818	0.4999	0.018*
C4	0.15350 (9)	0.51968 (15)	0.55294 (9)	0.0147 (3)
H4	0.0859	0.5217	0.5702	0.018*
C5	0.16945 (10)	0.67321 (16)	0.48659 (9)	0.0157 (3)
C6	0.09511 (9)	0.64834 (16)	0.39688 (9)	0.0161 (3)
C7	0.02301 (10)	0.76017 (17)	0.36135 (10)	0.0199 (3)
H7	0.0172	0.8623	0.3936	0.024*
C8	−0.04079 (10)	0.72243 (19)	0.27836 (11)	0.0242 (3)
H8	−0.0894	0.7994	0.2538	0.029*
C9	−0.03310 (10)	0.5725 (2)	0.23190 (10)	0.0252 (3)
H9	−0.0771	0.5464	0.1761	0.030*
C10	0.03931 (10)	0.45948 (19)	0.26700 (10)	0.0216 (3)
H10	0.0442	0.3568	0.2351	0.026*
C11	0.10405 (9)	0.49792 (17)	0.34867 (9)	0.0172 (3)
C12	0.18898 (10)	0.38987 (16)	0.39219 (9)	0.0167 (3)
C13	0.27923 (10)	0.49978 (16)	0.40301 (9)	0.0159 (3)
C14	0.36774 (10)	0.45997 (18)	0.37202 (10)	0.0206 (3)
H14	0.3746	0.3601	0.3379	0.025*
C15	0.44605 (10)	0.56721 (19)	0.39128 (10)	0.0253 (3)
H15	0.5065	0.5400	0.3704	0.030*
C16	0.43639 (10)	0.71368 (19)	0.44081 (10)	0.0239 (3)
H16	0.4903	0.7861	0.4534	0.029*
C17	0.34813 (10)	0.75541 (17)	0.47223 (10)	0.0195 (3)
H17	0.3417	0.8559	0.5059	0.023*
C18	0.26956 (10)	0.64801 (16)	0.45364 (9)	0.0159 (3)
C19	0.15742 (11)	0.83661 (16)	0.53834 (10)	0.0207 (3)
H19A	0.0939	0.8391	0.5618	0.031*
H19B	0.1619	0.9282	0.4932	0.031*
H19C	0.2087	0.8474	0.5932	0.031*
C20	0.19871 (11)	0.22982 (17)	0.33594 (10)	0.0230 (3)
H20A	0.2102	0.2562	0.2698	0.034*
H20B	0.1389	0.1654	0.3342	0.034*
H20C	0.2533	0.1654	0.3678	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0145 (6)	0.0179 (6)	0.0133 (5)	−0.0008 (4)	0.0005 (4)	0.0025 (4)
O1	0.0195 (5)	0.0236 (5)	0.0173 (5)	−0.0011 (4)	0.0024 (4)	−0.0065 (4)
O2	0.0259 (6)	0.0150 (5)	0.0245 (5)	0.0039 (4)	0.0045 (4)	0.0008 (4)
O3	0.0143 (5)	0.0250 (5)	0.0176 (5)	−0.0010 (4)	−0.0024 (4)	0.0058 (4)
C1	0.0129 (6)	0.0164 (7)	0.0159 (7)	−0.0034 (5)	0.0058 (5)	0.0010 (5)
C2	0.0182 (7)	0.0144 (7)	0.0167 (7)	−0.0036 (5)	0.0062 (5)	0.0021 (5)
C3	0.0149 (6)	0.0152 (7)	0.0154 (7)	−0.0028 (5)	0.0032 (5)	−0.0006 (5)
C4	0.0130 (6)	0.0160 (6)	0.0155 (7)	−0.0015 (5)	0.0031 (5)	−0.0010 (5)
C5	0.0154 (7)	0.0153 (7)	0.0166 (7)	−0.0006 (5)	0.0026 (5)	0.0010 (5)
C6	0.0141 (7)	0.0190 (7)	0.0158 (7)	−0.0024 (5)	0.0049 (5)	0.0024 (5)
C7	0.0173 (7)	0.0193 (7)	0.0242 (8)	0.0006 (5)	0.0067 (6)	0.0055 (6)
C8	0.0158 (7)	0.0310 (8)	0.0261 (8)	0.0008 (6)	0.0034 (6)	0.0126 (6)

C9	0.0193 (7)	0.0376 (9)	0.0177 (7)	−0.0065 (6)	−0.0011 (6)	0.0059 (6)
C10	0.0202 (7)	0.0280 (8)	0.0168 (7)	−0.0038 (6)	0.0026 (5)	−0.0007 (6)
C11	0.0167 (7)	0.0207 (7)	0.0149 (7)	−0.0026 (5)	0.0048 (5)	0.0019 (5)
C12	0.0187 (7)	0.0187 (7)	0.0130 (6)	−0.0008 (5)	0.0028 (5)	−0.0005 (5)
C13	0.0172 (7)	0.0194 (7)	0.0110 (6)	0.0013 (5)	0.0015 (5)	0.0048 (5)
C14	0.0218 (7)	0.0233 (7)	0.0179 (7)	0.0056 (6)	0.0072 (6)	0.0054 (6)
C15	0.0170 (7)	0.0350 (9)	0.0251 (8)	0.0061 (6)	0.0079 (6)	0.0138 (7)
C16	0.0159 (7)	0.0310 (8)	0.0242 (8)	−0.0048 (6)	0.0005 (6)	0.0118 (6)
C17	0.0198 (7)	0.0206 (7)	0.0175 (7)	−0.0030 (6)	−0.0003 (5)	0.0055 (6)
C18	0.0158 (7)	0.0189 (7)	0.0127 (6)	0.0011 (5)	0.0012 (5)	0.0051 (5)
C19	0.0229 (7)	0.0174 (7)	0.0223 (7)	0.0001 (6)	0.0046 (6)	−0.0011 (6)
C20	0.0292 (8)	0.0219 (7)	0.0181 (7)	0.0003 (6)	0.0039 (6)	−0.0034 (6)

Geometric parameters (Å, º)

N1—C1	1.3679 (17)	C9—H9	0.9500
N1—O3	1.3831 (14)	C10—C11	1.3933 (19)
N1—C2	1.3981 (17)	C10—H10	0.9500
O1—C1	1.2223 (16)	C11—C12	1.5314 (19)
O2—C2	1.2099 (16)	C12—C13	1.5304 (19)
O3—H3A	0.96 (2)	C12—C20	1.5308 (19)
C1—C4	1.5149 (18)	C13—C14	1.3936 (19)
C2—C3	1.5264 (18)	C13—C18	1.4085 (18)
C3—C4	1.5567 (17)	C14—C15	1.392 (2)
C3—C12	1.5758 (18)	C14—H14	0.9500
C3—H3	1.0000	C15—C16	1.388 (2)
C4—C5	1.5831 (18)	C15—H15	0.9500
C4—H4	1.0000	C16—C17	1.397 (2)
C5—C19	1.5275 (18)	C16—H16	0.9500
C5—C6	1.5303 (18)	C17—C18	1.3948 (19)
C5—C18	1.5345 (18)	C17—H17	0.9500
C6—C7	1.3944 (19)	C19—H19A	0.9800
C6—C11	1.4053 (19)	C19—H19B	0.9800
C7—C8	1.399 (2)	C19—H19C	0.9800
C7—H7	0.9500	C20—H20A	0.9800
C8—C9	1.387 (2)	C20—H20B	0.9800
C8—H8	0.9500	C20—H20C	0.9800
C9—C10	1.402 (2)		

C1—N1—O3	121.87 (10)	C11—C10—H10	120.0
C1—N1—C2	115.83 (11)	C9—C10—H10	120.0
O3—N1—C2	122.27 (11)	C10—C11—C6	119.83 (12)
N1—O3—H3A	100.7 (12)	C10—C11—C12	125.48 (12)
O1—C1—N1	123.07 (12)	C6—C11—C12	114.68 (11)
O1—C1—C4	129.30 (12)	C13—C12—C20	114.73 (11)
N1—C1—C4	107.62 (11)	C13—C12—C11	106.67 (11)
O2—C2—N1	123.39 (12)	C20—C12—C11	113.32 (11)
O2—C2—C3	130.24 (12)	C13—C12—C3	103.89 (10)
N1—C2—C3	106.36 (11)	C20—C12—C3	111.94 (11)
C2—C3—C4	104.88 (10)	C11—C12—C3	105.43 (10)

C2—C3—C12	111.78 (11)	C14—C13—C18	119.86 (13)
C4—C3—C12	110.94 (10)	C14—C13—C12	125.47 (12)
C2—C3—H3	109.7	C18—C13—C12	114.58 (11)
C4—C3—H3	109.7	C15—C14—C13	119.71 (13)
C12—C3—H3	109.7	C15—C14—H14	120.1
C1—C4—C3	104.90 (10)	C13—C14—H14	120.1
C1—C4—C5	112.69 (10)	C16—C15—C14	120.43 (13)
C3—C4—C5	110.51 (10)	C16—C15—H15	119.8
C1—C4—H4	109.5	C14—C15—H15	119.8
C3—C4—H4	109.5	C15—C16—C17	120.54 (13)
C5—C4—H4	109.5	C15—C16—H16	119.7
C19—C5—C6	113.39 (11)	C17—C16—H16	119.7
C19—C5—C18	114.55 (11)	C18—C17—C16	119.30 (13)
C6—C5—C18	106.32 (10)	C18—C17—H17	120.3
C19—C5—C4	111.91 (10)	C16—C17—H17	120.3
C6—C5—C4	104.10 (10)	C17—C18—C13	120.16 (12)
C18—C5—C4	105.72 (10)	C17—C18—C5	125.47 (12)
C7—C6—C11	119.84 (12)	C13—C18—C5	114.35 (11)
C7—C6—C5	125.74 (12)	C5—C19—H19A	109.5
C11—C6—C5	114.42 (11)	C5—C19—H19B	109.5
C6—C7—C8	120.17 (13)	H19A—C19—H19B	109.5
C6—C7—H7	119.9	C5—C19—H19C	109.5
C8—C7—H7	119.9	H19A—C19—H19C	109.5
C9—C8—C7	119.95 (13)	H19B—C19—H19C	109.5
C9—C8—H8	120.0	C12—C20—H20A	109.5
C7—C8—H8	120.0	C12—C20—H20B	109.5
C8—C9—C10	120.27 (13)	H20A—C20—H20B	109.5
C8—C9—H9	119.9	C12—C20—H20C	109.5
C10—C9—H9	119.9	H20A—C20—H20C	109.5
C11—C10—C9	119.92 (14)	H20B—C20—H20C	109.5

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C6–C11 ring. Cg2 refers to the mid-point of the C15—C16 bond.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O1^{i}	0.96 (2)	1.69 (2)	2.630 (1)	167 (2)
C8—H8···O1^{ii}	0.95	2.54	3.408 (2)	152
C15—H15···O3^{iii}	0.95	2.46	3.273 (2)	143
C17—H17···O2^{iv}	0.95	2.54	3.457 (2)	163
C4—H4···*Cg*1^{v}	1.00	2.66	3.518 (3)	144
C10—H10···*Cg*2^{vi}	0.95	2.77	3.668 (3)	158

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) *x*−1/2, −*y*+3/2, *z*−1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, *y*+1, *z*; (v) −*x*, −*y*+1, −*z*+1; (vi) −*x*+1/2, *y*−1/2, −*z*+1/2.