Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dihydroallocryptopine

Wenwen Sun, Yuyan Qin, Zhe Hou, Yao Yao and Le Zhou*

College of Science, Northwest Agriculture and Forestry University, Yangling 712100, People's Republic of China
Correspondence e-mail: zhoulechem@yahoo.com.cn

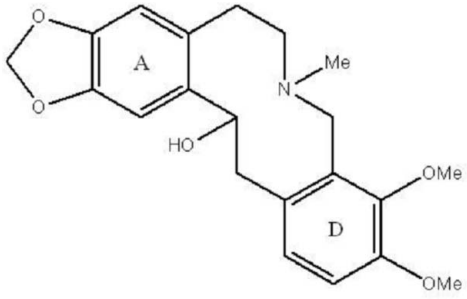
Received 12 November 2011; accepted 3 December 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.110; data-to-parameter ratio = 14.7.

In the title compound [systematic name: 7,8-dimethoxy-11-methyl-17,19-dioxa-11-azatetracyclo[12.7.0.0^{4,9}.0^{16,20}]henicosa-1(21),4,6,8,14,16 (20)-hexaen-2-ol], $C_{21}H_{25}NO_5$, the benzene rings are inclined at a dihedral angle of 23.16 (5)°. One of the methoxy C atoms is close to coplanar with its attached ring [deviation = 0.129 (3) Å], whereas the other is orientated away from the ring [deviation = −1.124 (2) Å]. The 10-membered ring is highly puckered, and the OH and CH_3 substituents project to the same side of the ring. In the crystal, O—H···O hydrogen bonds link the molecules into [010] chains and C—H···O and C—H···π interactions consolidate the packing.

Related literature

For the synthesis of the title compound, see: Wada *et al.* (2007). For the biological activity of allocryptopine derivatives, see: Morteza *et al.* (2003); Yan *et al.* (2009); Capasso *et al.* (1997); Jeong *et al.* (2009); Zhao *et al.* (2008). For a related structure, see: Valpuesta *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{25}NO_5$
M_r = 371.42
Monoclinic, $P2_1/c$
a = 14.2557 (19) Å
b = 9.3705 (13) Å
c = 15.278 (2) Å
β = 106.601 (2)°
V = 1955.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.45 × 0.24 × 0.21 mm

Data collection

Bruker SMART APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.981
14189 measured reflections
3646 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.02
3646 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*2 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O5^{i}	0.82	2.03	2.8380 (16)	168
C7—H7A···O4^{ii}	0.97	2.57	3.405 (3)	144
C18—H18···O3^{iii}	0.93	2.53	3.229 (2)	132
C7—H7B···$Cg2^{iv}$	0.97	2.57	3.464 (3)	153

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

This work was supported by the National Natural Science Foundation of China (NNSF; No. 31172365; 31101469).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6507).

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Yan, M., Sun, J. H., Lu, Z. Q., Chen, G. T., Guan, S. H., Liu, X., Jiang, B. H., Ye, M. & Guo, D. A. (2009). *J. Chromatogr. A*, **1216**, 2045–2062.
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supporting information

Acta Cryst. (2012). E**68**, o69 [doi:10.1107/S1600536811052172]

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S1. Comment

The allocryptopine derivatives have recently attracted great attention due to their antifungal activity (Morteza *et al.* 2003), antibacterial activity (Yan *et al.* 2009), analgesic effect (Capasso *et al.* 1997), anti-dementia (Jeong *et al.* 2009; Zhao *et al.* 2008), and so on. With the interests in the synthesis of allocryptopine derivatives with biological activity, we report here the synthesis and crystal structure of the title compound, (I).

As shown in Fig. 1, the molecule of the title compound is characterized by the presence of a ten-membered ring (hexahydrodibenzo*[c,g]*azecine) with a methylated tertiary nitrogen atom and a hydroxyl group fused to two aryl moieties. In general, the title compound have two oxygenated substituents on the benzene ring and two methoxyl on the other benzene ring. Benzene rings C1/C2/C3/C4/C5/C6 and C10/C11/C16/C17/C18/C19 are inclined with respect to one another with a dihedral angle of 23.16 (5)°.

In the crystal structure, two adjacent molecules are linked by weak intermolecular O—H···O or C—H···O hydrogen bond into a one-dimension chain along *b* axis. These chains are further connected by C—H···π interaction into two-dimension sheets.

S2. Experimental

The title compound was synthesized according to the literature procedure (Wada *et al.* 2007), and colourless blocks of (I) were obtained from a solution in methanol by slow evaporation at room temperature.

S3. Refinement

H atoms were positioned geometrically and treated as riding, with C—H bond lengths constrained to 0.93 (aromatic CH), or 0.97 Å (methylene CH_2), or 0.96Å (methyl CH_3), and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5Uc_{eq}(O)$.

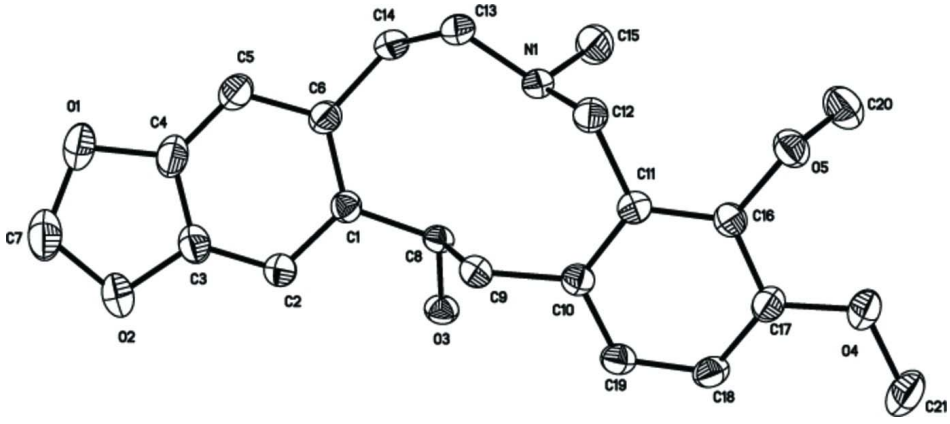

Figure 1

The molecular structure of the title compound (50% displacement ellipsoids).

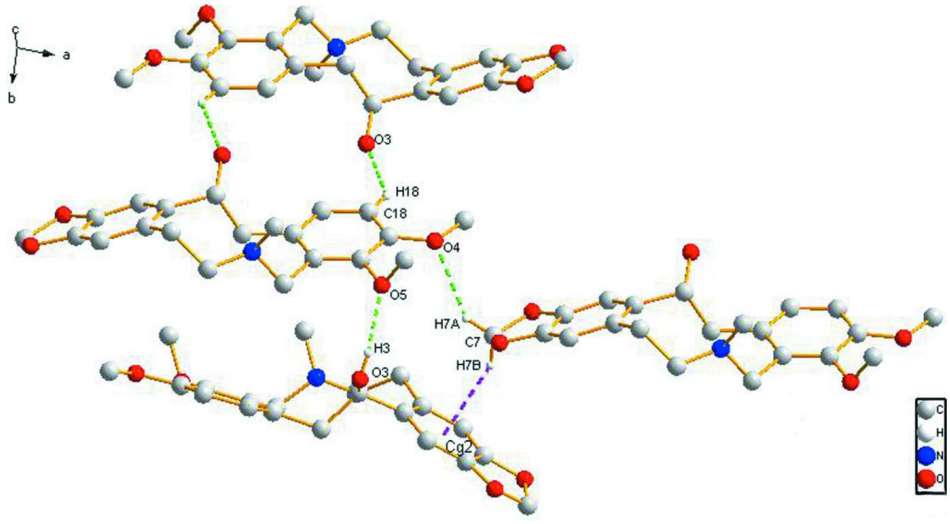

Figure 2

The two-dimension sheet structure of the title compound.

7,8-dimethoxy-11-methyl-17,19-dioxa-11- azatetracyclo[12.7.0.0^{4,9}.0^{16,20}]henicosa-1(21),4,6,8,14,16 (20)-hexaen-2-ol

Crystal data

$C_{21}H_{25}NO_5$
M_r = 371.42
Monoclinic, $P2_1/c$
a = 14.2557 (19) Å
b = 9.3705 (13) Å
c = 15.278 (2) Å
β = 106.601 (2)°
V = 1955.8 (5) Å^3
Z = 4
$F(000)$ = 792
D_x = 1.261 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3665 reflections
θ = 2.6–22.6°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.45 × 0.24 × 0.21 mm

Data collection

Bruker SMART APEX II CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.981
14189 measured reflections
3646 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.5°, θ_{min} = 2.6°
h = −17→17
k = −11→11
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.02
3646 reflections
248 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
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.4075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

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}
C1	0.27622 (11)	0.13752 (17)	0.24521 (10)	0.0402 (4)
C2	0.32459 (11)	0.17612 (18)	0.18061 (11)	0.0460 (4)
H2	0.2954	0.1612	0.1186	0.055*
C3	0.41532 (12)	0.2359 (2)	0.21064 (13)	0.0528 (4)
C4	0.46009 (13)	0.2568 (2)	0.30202 (14)	0.0592 (5)
C5	0.41615 (12)	0.2188 (2)	0.36684 (13)	0.0588 (5)
H5	0.4478	0.2329	0.4285	0.071*
C6	0.32187 (11)	0.15767 (19)	0.33900 (11)	0.0464 (4)
C7	0.55723 (15)	0.3447 (3)	0.22467 (16)	0.0776 (6)
H7A	0.6186	0.3106	0.2168	0.093*
H7B	0.5539	0.4471	0.2151	0.093*
C8	0.17251 (11)	0.08232 (16)	0.20842 (9)	0.0375 (3)

H8	0.1545	0.0280	0.2560	0.045*
C9	0.10207 (11)	0.20855 (17)	0.17812 (11)	0.0410 (4)
H9A	0.1234	0.2850	0.2221	0.049*
H9B	0.1079	0.2429	0.1200	0.049*
C10	−0.00464 (11)	0.17974 (16)	0.16778 (10)	0.0381 (3)
C11	−0.04578 (11)	0.20517 (16)	0.23982 (10)	0.0381 (3)
C12	0.01951 (11)	0.25595 (18)	0.33146 (11)	0.0444 (4)
H12A	0.0477	0.3479	0.3243	0.053*
H12B	−0.0189	0.2670	0.3742	0.053*
C13	0.19042 (11)	0.2073 (2)	0.42234 (11)	0.0507 (4)
H13A	0.1902	0.2099	0.4857	0.061*
H13B	0.1988	0.3042	0.4035	0.061*
C14	0.27663 (12)	0.1155 (2)	0.41377 (11)	0.0530 (5)
H14A	0.3274	0.1183	0.4717	0.064*
H14B	0.2544	0.0174	0.4034	0.064*
C15	0.06335 (14)	0.0326 (2)	0.40923 (13)	0.0650 (5)
H15A	0.1137	−0.0388	0.4255	0.098*
H15B	0.0059	−0.0073	0.3672	0.098*
H15C	0.0478	0.0646	0.4631	0.098*
C16	−0.14540 (11)	0.18373 (17)	0.22552 (10)	0.0410 (4)
C17	−0.20575 (11)	0.13956 (18)	0.14017 (11)	0.0452 (4)
C18	−0.16472 (12)	0.11260 (18)	0.07058 (11)	0.0463 (4)
H18	−0.2036	0.0809	0.0142	0.056*
C19	−0.06541 (12)	0.13279 (17)	0.08482 (10)	0.0430 (4)
H19	−0.0385	0.1143	0.0372	0.052*
C20	−0.22408 (15)	0.0958 (2)	0.33403 (14)	0.0674 (5)
H20A	−0.2690	0.0419	0.2868	0.101*
H20B	−0.2569	0.1293	0.3769	0.101*
H20C	−0.1700	0.0361	0.3650	0.101*
C21	−0.36808 (14)	0.0889 (3)	0.04815 (15)	0.0854 (7)
H21A	−0.3646	0.1587	0.0032	0.128*
H21B	−0.4337	0.0846	0.0529	0.128*
H21C	−0.3498	−0.0028	0.0303	0.128*
N1	0.09746 (9)	0.15187 (14)	0.36674 (8)	0.0403 (3)
O1	0.55278 (10)	0.3128 (2)	0.31403 (11)	0.0870 (5)
O2	0.47711 (10)	0.27719 (17)	0.16005 (10)	0.0764 (4)
O3	0.16204 (8)	−0.00602 (12)	0.12969 (7)	0.0458 (3)
H3	0.1735	−0.0892	0.1458	0.069*
O4	−0.30345 (8)	0.12764 (16)	0.13363 (8)	0.0642 (4)
O5	−0.18857 (8)	0.21548 (12)	0.29420 (7)	0.0497 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0378 (8)	0.0418 (9)	0.0418 (9)	0.0010 (7)	0.0127 (7)	−0.0015 (7)
C2	0.0419 (9)	0.0530 (10)	0.0431 (9)	0.0002 (7)	0.0121 (7)	0.0017 (7)
C3	0.0446 (10)	0.0587 (11)	0.0594 (11)	−0.0037 (8)	0.0216 (8)	0.0003 (9)
C4	0.0407 (9)	0.0668 (12)	0.0694 (12)	−0.0113 (9)	0.0147 (9)	−0.0111 (10)

C5	0.0432 (10)	0.0793 (14)	0.0511 (10)	−0.0077 (9)	0.0089 (8)	−0.0145 (9)
C6	0.0395 (9)	0.0553 (10)	0.0428 (9)	0.0013 (7)	0.0091 (7)	−0.0051 (8)
C7	0.0530 (12)	0.0853 (16)	0.0995 (17)	−0.0185 (11)	0.0298 (12)	−0.0081 (13)
C8	0.0417 (8)	0.0422 (9)	0.0301 (7)	−0.0026 (7)	0.0125 (6)	−0.0025 (6)
C9	0.0429 (9)	0.0425 (9)	0.0389 (8)	−0.0011 (7)	0.0140 (7)	0.0029 (7)
C10	0.0408 (8)	0.0357 (8)	0.0375 (8)	0.0027 (6)	0.0111 (6)	0.0027 (6)
C11	0.0407 (8)	0.0346 (8)	0.0381 (8)	0.0007 (6)	0.0095 (7)	−0.0015 (6)
C12	0.0430 (9)	0.0473 (9)	0.0436 (9)	−0.0029 (7)	0.0136 (7)	−0.0117 (7)
C13	0.0456 (9)	0.0690 (12)	0.0369 (8)	−0.0084 (8)	0.0108 (7)	−0.0137 (8)
C14	0.0440 (9)	0.0768 (13)	0.0347 (8)	−0.0011 (9)	0.0057 (7)	−0.0011 (8)
C15	0.0613 (11)	0.0714 (13)	0.0612 (12)	−0.0116 (10)	0.0156 (9)	0.0148 (10)
C16	0.0408 (8)	0.0424 (9)	0.0413 (9)	0.0025 (7)	0.0142 (7)	−0.0021 (7)
C17	0.0376 (9)	0.0493 (10)	0.0456 (9)	0.0016 (7)	0.0069 (7)	−0.0019 (7)
C18	0.0458 (9)	0.0531 (10)	0.0350 (8)	0.0012 (8)	0.0036 (7)	−0.0040 (7)
C19	0.0478 (9)	0.0462 (9)	0.0357 (8)	0.0048 (7)	0.0130 (7)	0.0005 (7)
C20	0.0694 (13)	0.0749 (14)	0.0672 (12)	−0.0005 (11)	0.0347 (10)	0.0095 (10)
C21	0.0436 (11)	0.128 (2)	0.0719 (14)	−0.0027 (12)	−0.0039 (10)	−0.0165 (14)
N1	0.0398 (7)	0.0478 (8)	0.0326 (6)	−0.0057 (6)	0.0095 (5)	−0.0040 (6)
O1	0.0522 (8)	0.1244 (14)	0.0852 (11)	−0.0369 (9)	0.0208 (7)	−0.0178 (10)
O2	0.0563 (8)	0.1040 (12)	0.0760 (9)	−0.0229 (8)	0.0303 (7)	0.0018 (8)
O3	0.0541 (7)	0.0482 (7)	0.0363 (6)	−0.0031 (6)	0.0150 (5)	−0.0074 (5)
O4	0.0363 (6)	0.0958 (10)	0.0561 (7)	−0.0040 (6)	0.0062 (5)	−0.0098 (7)
O5	0.0496 (7)	0.0551 (7)	0.0499 (7)	−0.0007 (5)	0.0229 (5)	−0.0060 (5)

Geometric parameters (Å, º)

C1—C2	1.403 (2)	C12—H12B	0.9700
C1—C6	1.407 (2)	C13—N1	1.4506 (19)
C1—C8	1.515 (2)	C13—C14	1.536 (2)
C2—C3	1.363 (2)	C13—H13A	0.9700
C2—H2	0.9300	C13—H13B	0.9700
C3—C4	1.373 (3)	C14—H14A	0.9700
C3—O2	1.383 (2)	C14—H14B	0.9700
C4—C5	1.362 (3)	C15—N1	1.445 (2)
C4—O1	1.384 (2)	C15—H15A	0.9600
C5—C6	1.410 (2)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600
C6—C14	1.516 (2)	C16—O5	1.3920 (18)
C7—O1	1.417 (3)	C16—C17	1.404 (2)
C7—O2	1.427 (2)	C17—O4	1.3720 (19)
C7—H7A	0.9700	C17—C18	1.375 (2)
C7—H7B	0.9700	C18—C19	1.383 (2)
C8—O3	1.4323 (17)	C18—H18	0.9300
C8—C9	1.535 (2)	C19—H19	0.9300
C8—H8	0.9800	C20—O5	1.435 (2)
C9—C10	1.508 (2)	C20—H20A	0.9600
C9—H9A	0.9700	C20—H20B	0.9600
C9—H9B	0.9700	C20—H20C	0.9600

C10—C19	1.387 (2)	C21—O4	1.414 (2)
C10—C11	1.407 (2)	C21—H21A	0.9600
C11—C16	1.388 (2)	C21—H21B	0.9600
C11—C12	1.519 (2)	C21—H21C	0.9600
C12—N1	1.461 (2)	O3—H3	0.8200
C12—H12A	0.9700		

C2—C1—C6	120.30 (14)	N1—C13—H13A	109.3
C2—C1—C8	116.79 (13)	C14—C13—H13A	109.3
C6—C1—C8	122.82 (13)	N1—C13—H13B	109.3
C3—C2—C1	118.61 (15)	C14—C13—H13B	109.3
C3—C2—H2	120.7	H13A—C13—H13B	108.0
C1—C2—H2	120.7	C6—C14—C13	116.17 (15)
C2—C3—C4	121.44 (16)	C6—C14—H14A	108.2
C2—C3—O2	128.43 (17)	C13—C14—H14A	108.2
C4—C3—O2	110.06 (15)	C6—C14—H14B	108.2
C5—C4—C3	121.68 (16)	C13—C14—H14B	108.2
C5—C4—O1	128.52 (18)	H14A—C14—H14B	107.4
C3—C4—O1	109.74 (17)	N1—C15—H15A	109.5
C4—C5—C6	118.93 (16)	N1—C15—H15B	109.5
C4—C5—H5	120.5	H15A—C15—H15B	109.5
C6—C5—H5	120.5	N1—C15—H15C	109.5
C1—C6—C5	119.03 (15)	H15A—C15—H15C	109.5
C1—C6—C14	124.04 (14)	H15B—C15—H15C	109.5
C5—C6—C14	116.92 (14)	C11—C16—O5	120.21 (13)
O1—C7—O2	109.03 (15)	C11—C16—C17	121.11 (14)
O1—C7—H7A	109.9	O5—C16—C17	118.53 (13)
O2—C7—H7A	109.9	O4—C17—C18	125.15 (14)
O1—C7—H7B	109.9	O4—C17—C16	115.57 (14)
O2—C7—H7B	109.9	C18—C17—C16	119.28 (14)
H7A—C7—H7B	108.3	C17—C18—C19	119.72 (14)
O3—C8—C1	111.43 (12)	C17—C18—H18	120.1
O3—C8—C9	106.85 (12)	C19—C18—H18	120.1
C1—C8—C9	109.50 (13)	C18—C19—C10	122.10 (14)
O3—C8—H8	109.7	C18—C19—H19	118.9
C1—C8—H8	109.7	C10—C19—H19	118.9
C9—C8—H8	109.7	O5—C20—H20A	109.5
C10—C9—C8	116.55 (13)	O5—C20—H20B	109.5
C10—C9—H9A	108.2	H20A—C20—H20B	109.5
C8—C9—H9A	108.2	O5—C20—H20C	109.5
C10—C9—H9B	108.2	H20A—C20—H20C	109.5
C8—C9—H9B	108.2	H20B—C20—H20C	109.5
H9A—C9—H9B	107.3	O4—C21—H21A	109.5
C19—C10—C11	118.51 (14)	O4—C21—H21B	109.5
C19—C10—C9	120.04 (13)	H21A—C21—H21B	109.5
C11—C10—C9	121.40 (13)	O4—C21—H21C	109.5
C16—C11—C10	119.24 (13)	H21A—C21—H21C	109.5
C16—C11—C12	121.34 (13)	H21B—C21—H21C	109.5

C10—C11—C12	119.42 (13)	C15—N1—C13	112.48 (14)
N1—C12—C11	109.40 (12)	C15—N1—C12	111.35 (14)
N1—C12—H12A	109.8	C13—N1—C12	116.64 (13)
C11—C12—H12A	109.8	C4—O1—C7	104.83 (15)
N1—C12—H12B	109.8	C3—O2—C7	104.43 (15)
C11—C12—H12B	109.8	C8—O3—H3	109.5
H12A—C12—H12B	108.2	C17—O4—C21	117.92 (14)
N1—C13—C14	111.64 (14)	C16—O5—C20	115.97 (13)

C6—C1—C2—C3	−1.3 (2)	C1—C6—C14—C13	−71.7 (2)
C8—C1—C2—C3	175.33 (15)	C5—C6—C14—C13	109.25 (18)
C1—C2—C3—C4	0.9 (3)	N1—C13—C14—C6	90.26 (18)
C1—C2—C3—O2	177.59 (17)	C10—C11—C16—O5	−176.56 (13)
C2—C3—C4—C5	0.1 (3)	C12—C11—C16—O5	3.2 (2)
O2—C3—C4—C5	−177.16 (18)	C10—C11—C16—C17	−1.1 (2)
C2—C3—C4—O1	177.33 (17)	C12—C11—C16—C17	178.70 (15)
O2—C3—C4—O1	0.1 (2)	C11—C16—C17—O4	−177.48 (14)
C3—C4—C5—C6	−0.6 (3)	O5—C16—C17—O4	−1.9 (2)
O1—C4—C5—C6	−177.3 (2)	C11—C16—C17—C18	2.2 (2)
C2—C1—C6—C5	0.8 (3)	O5—C16—C17—C18	177.73 (14)
C8—C1—C6—C5	−175.64 (15)	O4—C17—C18—C19	177.98 (16)
C2—C1—C6—C14	−178.21 (16)	C16—C17—C18—C19	−1.7 (2)
C8—C1—C6—C14	5.3 (3)	C17—C18—C19—C10	0.1 (3)
C4—C5—C6—C1	0.2 (3)	C11—C10—C19—C18	1.0 (2)
C4—C5—C6—C14	179.25 (17)	C9—C10—C19—C18	−176.33 (15)
C2—C1—C8—O3	38.31 (19)	C14—C13—N1—C15	79.54 (18)
C6—C1—C8—O3	−145.11 (15)	C14—C13—N1—C12	−150.04 (14)
C2—C1—C8—C9	−79.68 (17)	C11—C12—N1—C15	−80.48 (17)
C6—C1—C8—C9	96.90 (17)	C11—C12—N1—C13	148.58 (13)
O3—C8—C9—C10	77.80 (16)	C5—C4—O1—C7	−174.7 (2)
C1—C8—C9—C10	−161.39 (13)	C3—C4—O1—C7	8.3 (2)
C8—C9—C10—C19	−89.37 (18)	O2—C7—O1—C4	−13.5 (2)
C8—C9—C10—C11	93.35 (17)	C2—C3—O2—C7	174.7 (2)
C19—C10—C11—C16	−0.5 (2)	C4—C3—O2—C7	−8.3 (2)
C9—C10—C11—C16	176.82 (14)	O1—C7—O2—C3	13.6 (2)
C19—C10—C11—C12	179.70 (14)	C18—C17—O4—C21	−2.1 (3)
C9—C10—C11—C12	−3.0 (2)	C16—C17—O4—C21	177.58 (18)
C16—C11—C12—N1	121.81 (15)	C11—C16—O5—C20	−112.30 (17)
C10—C11—C12—N1	−58.39 (19)	C17—C16—O5—C20	72.12 (19)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O5^{i}	0.82	2.03	2.8380 (16)	168
C7—H7*A*···O4^{ii}	0.97	2.57	3.405 (3)	144

C18—H18···O3^{iii}	0.93	2.53	3.229 (2)	132
C7—H7*B*···*Cg*2^{iv}	0.97	2.57	3.464 (3)	153

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