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(3*R*,3a*S*,6*R*,6a*R*)-*tert*-Butyl *N*-(6-chloro-2-oxo-6a-phenylperhydrofuro[3,2-*b*]-furan-3-yl)carbamate

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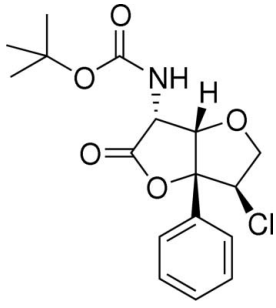
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.079; data-to-parameter ratio = 14.8.

The chiral title compound, $C_{17}H_{20}ClNO_5$, arose as a side product during the synthesis of novel furanomycin derivatives. The stereochemistry at the bicyclic core is consistent with a halolactonization step. The five-membered rings are nearly perpendicular to each other [torsion angle at the common bond: −88.3 (3)°].

Related literature

For related literature, see: Erdsack & Krause (2007); Erdsack *et al.* (2007); Hoffmann-Röder & Krause (2001).



Experimental

Crystal data

$C_{17}H_{20}ClNO_5$
M_r = 353.79
Orthorhombic, $P2_12_12_1$
a = 6.1519 (7) Å
b = 12.029 (2) Å
c = 23.655 (4) Å
V = 1750.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 291 (1) K
0.44 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
14042 measured reflections
3280 independent reflections
1085 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.079
S = 1.01
3280 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Absolute structure: Flack (1983), with 1313 Friedel pairs
Flack parameter: 0.08 (10)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2449).

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supplementary materials

Acta Cryst. (2007). E**63**, o3371 [**doi:10.1107/S1600536807031388**]

(3*R*,3a*S*,6*R*,6a*R*)-*tert*-Butyl *N*-(6-chloro-2-oxo-6a-phenylperhydrofuro[3,2-*b*]furan-3-yl)carbamate

J. Erdsack, M. Schürmann, H. Preut and N. Krause

Comment

The title compound, (I), is a side product in the preparation of novel furanomycin derivatives using the gold-catalyzed cyclization of α-hydroxyallenes (Hoffmann-Röder & Krause, 2001). It was obtained after an aldehyde oxidation in the presence of $NaClO_2$ and chlorolactonization of the resulted boc-protected amino acid intermediate by hypochloric acid, a degradation product of the oxidant (Erdsack & Krause, 2007). A crystal structure determination of (I) has now been carried out to establish the relative configuration of the stereogenic centers at the bicyclic core. Fig. 1 shows that the relative configuration of C6 and C6a is consistent with the stereospecific halolactonization step. The torsion angle O3—C7—C10—O1 is −88.3 (3)°. The configurations of the stereogenic C atoms in (I) (C3 *R*, C3a S, C6 *R* and C6a *R*) were established by refining the Flack (1983) absolute structure parameter; they are consistent with those of the equivalent atoms in the starting material (Erdsack *et al.*, 2007).

Experimental

In a Schlenk tube equipped with a magnetic stirrer bar, 47 mg (0.15 mmol) of *tert*-butyl-(1*R*,2S)-[2-hydroxy-1-(3-phenyl-2,5-dihydrofuran-2-yl)-ethyl]-carbamate (synthesis of this compound will be described elsewhere; Erdsack & Krause 2007) was dissolved in dry dichloromethane (1.5 ml) under argon and cooled to 273 K. With stirring, 87 mg (0.23 mmol) of Dess-Martin periodinane was added in one portion. After 2 h, the mixture was diluted with diethyl ether (3 ml), quenched with sat. aq. $NaHCO_3$ and sat. aq. $Na_2S_2O_3$ 1:1 (5 ml) and diluted with additional 3 ml of diethyl ether. After a few minutes with stirring at r.t., the biphasic mixture came clear. The organic phase was separated and the residue was extracted with diethyl ether (3 × 10 ml). The combined organic layers were washed with aq. sat. $NaHCO_3$ and brine and dried with $MgSO_4$. The solution was filtered and the solvent was evaporated. The crude aldehyde was dissolved in a 1:1 mixture of t-BuOH/THF (5 ml). The flask was sealed with a rubber septum and was cooled to 273 K. With vigorous stirring, a solution of $NaClO_2$ (80%, technical grade, 52 mg, 0.46 mmol) and NaH_2PO_4*H_2O (82 mg, 0.46 mmol) in 1 ml water was slowly added dropwise *via* syringe over 30 min. The reaction mixture came yellow and was allowed to stir at r.t. overnight. The mixture was diluted with water (15 ml) and extracted with diethyl ether (3 × 15 ml). The combined organic layers were dried ($MgSO_4$), filtered and the solvent was evaporated. The residue was purified by column chromatography on silica gel (iso-hexane/EtOAc 4:1 *v*/*v*) to give 28 mg (53%) of the lactone (I) as a solid, which was suspended in a few drops of iso-hexane. Ethyl acetate was added dropwise until the compound was completely dissolved, and colourless needles of (I) were obtained by slow evaporation at ambient temperature; mp 432 K; $[\alpha]_D^{21}$ − 44.0 (c 1.40, $CHCl_3$); IR (KBr pellet), cm^{-1}: 3419 (*m*), 3323 (*m*), 3062 (w), 2979 (*m*), 2932 (*m*), 2885 (w), 1801 (*s*), 1712 (*s*), 1510 (*m*), 1451 (*m*), 1393 (*m*), 1368 (*m*), 1253 (*m*), 1163 (*s*), 1104 (*m*), 1062 (*m*), 942 (*s*), 865 (*m*), 751 (*m*), 734 (*m*), 699 (*m*), 665 (w), 577 (w), 514 (w); ^{1}H NMR (400 MHz, $CDCl_3$): δ (p.p.m.): 7.48 − 7.43 (m, 5 H), 5.22 (dd, J = 6.3, 13.6 Hz, 1 H), 4.69 (dd, J = 4.0, 8.6 Hz, 1 H), 4.62 (d, J = 3.4 Hz, 1 H), 4.51 (dd, J = 3.9, 10.5 Hz, 1 H), 4.32 (d, J = 10.5 Hz, 1 H), 1.46 (m, 9 H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (p.p.m.) 172.0,

155.2, 132.1, 129.8, 128.7, 127.0, 94.8, 81.0, 80.1, 76.9, 63.3, 54.1, 28.2 HRMS (ESI): m/*z* calculated for $C_{17}H_{21}O_5N^{35}Cl$: $[M + H]^+$ = 354.11028, found 354.11002

Refinement

The H atoms were placed in calculated positions, with C—H = 0.93–0.98 and N—H = 0.86 Å and were refined as riding, with $U_{iso}(H) = 1.5U_{eq}$; the methyl groups were allowed to rotate but not to tip.

Figures

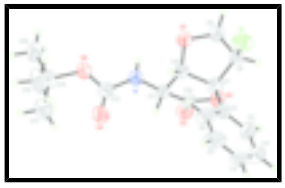


Fig. 1. : The molecular structure of (I) with displacement ellipsoids shown at the 30% probability level (arbitrary spheres for the H atoms).

(3*R*,3aS,6*R*,6aR)-*tert*-Butyl *N*-(6-chloro-2-oxo-6a-phenylperhydrofuro[3,2-*b*]furan-3-yl)carbamate

Crystal data

$C_{17}H_{20}ClNO_5$	F_{000} = 744
M_r = 353.79	D_x = 1.342 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 14042 reflections
a = 6.1519 (7) Å	θ = 3.1–25.8º
b = 12.029 (2) Å	μ = 0.24 mm^{-1}
c = 23.655 (4) Å	*T* = 291 (1) K
V = 1750.5 (5) Å^3	Needle, colourless
Z = 4	0.44 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer	3280 independent reflections
Radiation source: fine-focus sealed tube	1085 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
Detector resolution: 19 vertical, 18 horizontal pixels mm^{-1}	θ_{max} = 25.8º
T = 291(1) K	θ_{min} = 3.1º
309 frames via ω–rotation (Δω=1%) and two times 120 s per frame (three sets at different κ–angles) scans	*h* = −7→7
Absorption correction: none	*k* = 0→14
14042 measured reflections	*l* = 0→28

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$[1.0\exp(7.10(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2)]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.079$	$\Delta\rho_{max} = 0.10$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.11$ e Å^{-3}
3280 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
221 parameters	Extinction coefficient: 0.0215 (9)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1313 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.08 (10)
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl	0.6643 (2)	0.59959 (10)	0.85442 (5)	0.1028 (4)
O1	0.5371 (4)	0.6930 (2)	0.97543 (10)	0.0741 (7)
O2	0.0232 (4)	0.5437 (2)	1.04297 (11)	0.0772 (8)
O3	0.1997 (4)	0.5179 (2)	0.96171 (11)	0.0702 (7)
O4	0.5678 (5)	0.4974 (2)	1.14730 (11)	0.0925 (9)
O5	0.5498 (4)	0.6773 (2)	1.17002 (11)	0.0832 (8)
N	0.4380 (4)	0.6243 (2)	1.08588 (12)	0.0678 (8)
H0	0.3938	0.6917	1.0822	0.102*
C1	0.4893 (6)	0.4053 (3)	0.92572 (15)	0.0687 (10)
C2	0.3421 (8)	0.3404 (4)	0.89794 (16)	0.0938 (14)
H2	0.2048	0.3681	0.8894	0.141*
C3	0.3975 (9)	0.2339 (4)	0.88258 (19)	0.1040 (17)
H3	0.2977	0.1897	0.8635	0.156*
C4	0.5945 (10)	0.1938 (4)	0.8950 (2)	0.1002 (16)
H4	0.6314	0.1219	0.8843	0.150*
C5	0.7399 (9)	0.2570 (4)	0.9230 (2)	0.1152 (18)

H5	0.8761	0.2281	0.9317	0.173*
C6	0.6885 (8)	0.3633 (4)	0.93866 (18)	0.0982 (14)
H6	0.7891	0.4066	0.9581	0.147*
C7	0.4274 (6)	0.5205 (3)	0.94081 (14)	0.0601 (10)
C8	0.4180 (6)	0.6041 (3)	0.89390 (14)	0.0701 (10)
H8	0.2905	0.5928	0.8697	0.105*
C9	0.4034 (6)	0.7103 (3)	0.92654 (15)	0.0781 (12)
H9A	0.4570	0.7721	0.9042	0.117*
H9B	0.2543	0.7254	0.9375	0.117*
C10	0.5502 (5)	0.5787 (3)	0.98781 (15)	0.0626 (10)
H10	0.7011	0.5530	0.9906	0.094*
C11	0.4212 (5)	0.5507 (3)	1.03969 (15)	0.0649 (10)
H11	0.4684	0.4772	1.0527	0.097*
C12	0.1912 (7)	0.5391 (3)	1.01752 (18)	0.0662 (10)
C13	0.5233 (6)	0.5907 (4)	1.13647 (18)	0.0727 (11)
C14	0.6347 (7)	0.6647 (4)	1.22849 (16)	0.0861 (13)
C15	0.8603 (6)	0.6207 (5)	1.22662 (17)	0.132 (2)
H15A	0.9223	0.6230	1.2638	0.199*
H15B	0.9462	0.6653	1.2015	0.199*
H15C	0.8581	0.5453	1.2133	0.199*
C16	0.6267 (10)	0.7804 (4)	1.24998 (17)	0.156 (3)
H16A	0.4821	0.8091	1.2458	0.234*
H16B	0.7263	0.8257	1.2289	0.234*
H16C	0.6667	0.7813	1.2892	0.234*
C17	0.4855 (7)	0.5924 (4)	1.26134 (17)	0.1118 (15)
H17A	0.3408	0.6221	1.2596	0.168*
H17B	0.5325	0.5896	1.3000	0.168*
H17C	0.4866	0.5188	1.2456	0.168*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.1244 (9)	0.0872 (8)	0.0967 (8)	0.0053 (8)	0.0295 (7)	0.0076 (7)
O1	0.0901 (18)	0.0578 (18)	0.0744 (18)	−0.0033 (16)	−0.0172 (15)	0.0027 (13)
O2	0.0676 (17)	0.0769 (19)	0.0872 (19)	0.0014 (16)	−0.0038 (15)	0.0033 (15)
O3	0.0584 (16)	0.0840 (19)	0.0682 (17)	0.0018 (16)	−0.0079 (14)	−0.0048 (14)
O4	0.126 (2)	0.0707 (19)	0.0810 (19)	0.0217 (19)	−0.0200 (18)	0.0004 (17)
O5	0.112 (2)	0.0692 (19)	0.0681 (17)	−0.0006 (18)	−0.0191 (16)	0.0014 (15)
N	0.080 (2)	0.059 (2)	0.0639 (19)	0.0043 (18)	−0.0168 (17)	0.0010 (17)
C1	0.069 (3)	0.065 (3)	0.073 (3)	0.001 (3)	−0.002 (2)	0.000 (2)
C2	0.107 (4)	0.085 (3)	0.089 (3)	0.003 (3)	−0.019 (3)	−0.018 (3)
C3	0.130 (5)	0.085 (4)	0.096 (3)	−0.016 (3)	−0.008 (3)	−0.017 (3)
C4	0.143 (5)	0.059 (3)	0.099 (4)	0.003 (4)	0.015 (4)	0.003 (3)
C5	0.111 (5)	0.071 (4)	0.163 (5)	0.015 (3)	−0.013 (4)	0.013 (4)
C6	0.093 (3)	0.058 (3)	0.144 (4)	0.007 (3)	−0.016 (3)	−0.009 (3)
C7	0.054 (2)	0.056 (3)	0.070 (3)	0.003 (2)	−0.004 (2)	−0.001 (2)
C8	0.074 (2)	0.069 (3)	0.067 (2)	0.007 (3)	−0.004 (2)	0.004 (2)
C9	0.091 (3)	0.068 (3)	0.076 (3)	0.006 (2)	−0.016 (3)	0.004 (2)

C10	0.059 (2)	0.058 (3)	0.070 (2)	0.000 (2)	−0.004 (2)	−0.001 (2)
C11	0.064 (2)	0.061 (3)	0.070 (2)	−0.002 (2)	−0.016 (2)	−0.006 (2)
C12	0.062 (3)	0.057 (3)	0.079 (3)	0.000 (2)	−0.008 (3)	0.000 (2)
C13	0.068 (3)	0.075 (3)	0.075 (3)	0.001 (3)	−0.001 (2)	−0.002 (3)
C14	0.107 (4)	0.099 (4)	0.053 (3)	−0.004 (3)	−0.018 (3)	0.010 (2)
C15	0.085 (3)	0.220 (6)	0.092 (3)	0.000 (4)	−0.021 (3)	0.021 (4)
C16	0.279 (8)	0.100 (4)	0.088 (4)	−0.015 (5)	−0.055 (5)	−0.023 (3)
C17	0.112 (3)	0.146 (4)	0.078 (3)	0.005 (4)	0.009 (3)	0.010 (3)

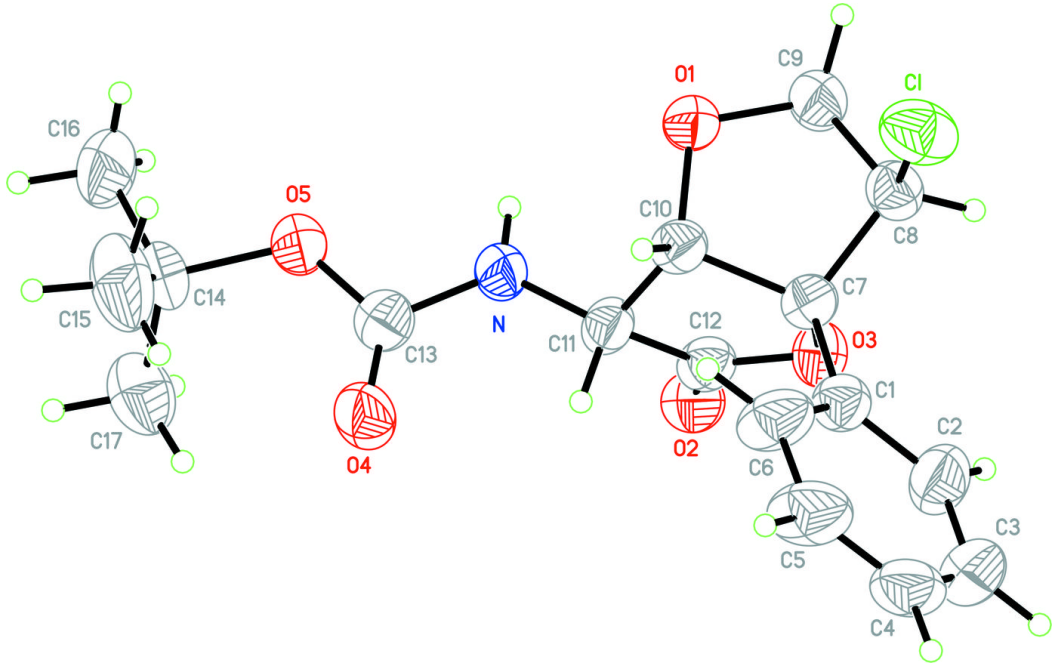
Geometric parameters (Å, °)

Cl—C8	1.781 (3)	C6—H6	0.9300
O1—C10	1.409 (4)	C7—C8	1.499 (4)
O1—C9	1.434 (4)	C7—C10	1.516 (4)
O2—C12	1.197 (4)	C8—C9	1.496 (5)
O3—C12	1.346 (4)	C8—H8	0.9800
O3—C7	1.486 (4)	C9—H9A	0.9700
O4—C13	1.183 (4)	C9—H9B	0.9700
O5—C13	1.320 (4)	C10—C11	1.500 (4)
O5—C14	1.486 (4)	C10—H10	0.9800
N—C13	1.368 (4)	C11—C12	1.516 (5)
N—C11	1.410 (4)	C11—H11	0.9800
N—H0	0.8600	C14—C16	1.483 (5)
C1—C6	1.360 (5)	C14—C17	1.484 (5)
C1—C2	1.364 (5)	C14—C15	1.486 (5)
C1—C7	1.481 (5)	C15—H15A	0.9600
C2—C3	1.374 (6)	C15—H15B	0.9600
C2—H2	0.9300	C15—H15C	0.9600
C3—C4	1.337 (6)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C5	1.347 (6)	C16—H16C	0.9600
C4—H4	0.9300	C17—H17A	0.9600
C5—C6	1.369 (5)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C10—O1—C9	110.0 (3)	O1—C10—C11	111.0 (3)
C12—O3—C7	111.0 (3)	O1—C10—C7	105.6 (3)
C13—O5—C14	121.5 (3)	C11—C10—C7	103.5 (3)
C13—N—C11	121.4 (3)	O1—C10—H10	112.1
C13—N—H0	119.3	C11—C10—H10	112.1
C11—N—H0	119.3	C7—C10—H10	112.1
C6—C1—C2	119.6 (4)	N—C11—C10	117.0 (3)
C6—C1—C7	121.6 (4)	N—C11—C12	113.2 (3)
C2—C1—C7	118.7 (4)	C10—C11—C12	103.4 (3)
C1—C2—C3	119.7 (5)	N—C11—H11	107.6
C1—C2—H2	120.1	C10—C11—H11	107.6
C3—C2—H2	120.1	C12—C11—H11	107.6
C4—C3—C2	120.2 (5)	O2—C12—O3	122.4 (3)
C4—C3—H3	119.9	O2—C12—C11	128.9 (4)
C2—C3—H3	119.9	O3—C12—C11	108.7 (4)

C3—C4—C5	120.4 (5)	O4—C13—O5	126.2 (4)
C3—C4—H4	119.8	O4—C13—N	123.9 (4)
C5—C4—H4	119.8	O5—C13—N	109.9 (4)
C4—C5—C6	120.4 (5)	C16—C14—C17	110.5 (4)
C4—C5—H5	119.8	C16—C14—O5	102.2 (3)
C6—C5—H5	119.8	C17—C14—O5	109.3 (3)
C1—C6—C5	119.6 (5)	C16—C14—C15	112.0 (4)
C1—C6—H6	120.2	C17—C14—C15	112.6 (4)
C5—C6—H6	120.2	O5—C14—C15	109.7 (3)
C1—C7—O3	107.6 (3)	C14—C15—H15A	109.5
C1—C7—C8	117.4 (3)	C14—C15—H15B	109.5
O3—C7—C8	102.9 (3)	H15A—C15—H15B	109.5
C1—C7—C10	118.7 (3)	C14—C15—H15C	109.5
O3—C7—C10	103.6 (3)	H15A—C15—H15C	109.5
C8—C7—C10	104.6 (3)	H15B—C15—H15C	109.5
C7—C8—C9	101.1 (3)	C14—C16—H16A	109.5
C7—C8—Cl	109.6 (3)	C14—C16—H16B	109.5
C9—C8—Cl	110.3 (3)	H16A—C16—H16B	109.5
C7—C8—H8	111.8	C14—C16—H16C	109.5
C9—C8—H8	111.8	H16A—C16—H16C	109.5
Cl—C8—H8	111.8	H16B—C16—H16C	109.5
O1—C9—C8	105.0 (3)	C14—C17—H17A	109.5
O1—C9—H9A	110.8	C14—C17—H17B	109.5
C8—C9—H9A	110.8	H17A—C17—H17B	109.5
O1—C9—H9B	110.8	C14—C17—H17C	109.5
C8—C9—H9B	110.8	H17A—C17—H17C	109.5
H9A—C9—H9B	108.8	H17B—C17—H17C	109.5
C6—C1—C2—C3	−0.9 (6)	C9—O1—C10—C7	3.9 (4)
C7—C1—C2—C3	178.8 (4)	C1—C7—C10—O1	152.5 (3)
C1—C2—C3—C4	0.3 (7)	O3—C7—C10—O1	−88.3 (3)
C2—C3—C4—C5	0.4 (8)	C8—C7—C10—O1	19.3 (4)
C3—C4—C5—C6	−0.5 (8)	C1—C7—C10—C11	−90.8 (4)
C2—C1—C6—C5	0.9 (7)	O3—C7—C10—C11	28.5 (3)
C7—C1—C6—C5	−178.8 (4)	C8—C7—C10—C11	136.0 (3)
C4—C5—C6—C1	−0.2 (8)	C13—N—C11—C10	−116.8 (4)
C6—C1—C7—O3	−138.5 (4)	C13—N—C11—C12	123.1 (4)
C2—C1—C7—O3	41.8 (4)	O1—C10—C11—N	−42.8 (4)
C6—C1—C7—C8	106.1 (5)	C7—C10—C11—N	−155.7 (3)
C2—C1—C7—C8	−73.6 (5)	O1—C10—C11—C12	82.5 (4)
C6—C1—C7—C10	−21.4 (5)	C7—C10—C11—C12	−30.4 (4)
C2—C1—C7—C10	158.9 (4)	C7—O3—C12—O2	178.3 (3)
C12—O3—C7—C1	110.8 (3)	C7—O3—C12—C11	−3.7 (4)
C12—O3—C7—C8	−124.7 (3)	N—C11—C12—O2	−32.6 (6)
C12—O3—C7—C10	−15.9 (4)	C10—C11—C12—O2	−160.2 (4)
C1—C7—C8—C9	−167.4 (3)	N—C11—C12—O3	149.5 (3)
O3—C7—C8—C9	74.6 (3)	C10—C11—C12—O3	21.9 (4)
C10—C7—C8—C9	−33.4 (4)	C14—O5—C13—O4	−2.5 (7)
C1—C7—C8—Cl	−50.9 (4)	C14—O5—C13—N	178.3 (3)
O3—C7—C8—Cl	−168.9 (2)	C11—N—C13—O4	−7.9 (6)

C10—C7—C8—Cl	83.1 (3)	C11—N—C13—O5	171.3 (3)
C10—O1—C9—C8	−25.6 (4)	C13—O5—C14—C16	−177.6 (4)
C7—C8—C9—O1	36.0 (4)	C13—O5—C14—C17	−60.5 (5)
Cl—C8—C9—O1	−79.9 (3)	C13—O5—C14—C15	63.4 (5)
C9—O1—C10—C11	−107.7 (3)		

Fig. 1


C16
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